

CHARACTERIZATION OF SELF-ADJOINT EXTENSIONS FOR DISCRETE SYMPLECTIC SYSTEMS

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ABSTRACT. All self-adjoint extensions of minimal linear relation associated with the discrete symplectic system are characterized. Especially, for the scalar case on a finite discrete interval some equivalent forms and the uniqueness of the given expression are discussed and the Krein–von Neumann extension is described explicitly. In addition, a limit point criterion for symplectic systems is established. The result partially generalizes even a classical limit point criterion for the second order Sturm–Liouville difference equations.

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1. INTRODUCTION

This paper is devoted to the characterization of all self-adjoint extensions of the minimal linear relation associated with the discrete symplectic system

$$z_k(\lambda) = \mathbb{S}_k(\lambda) z_{k+1}(\lambda), \quad \mathbb{S}_k(\lambda) := \mathcal{S}_k + \lambda \mathcal{V}_k, \quad (\mathbf{S}_\lambda)$$

where $\lambda \in \mathbb{C}$ is the spectral parameter, \mathcal{S}_k and \mathcal{V}_k are $2n \times 2n$ complex-valued matrices such that

$$\mathcal{S}_k^* \mathcal{J} \mathcal{S}_k = \mathcal{J}, \quad \mathcal{V}_k^* \mathcal{J} \mathcal{S}_k \text{ is Hermitian}, \quad \mathcal{V}_k^* \mathcal{J} \mathcal{V}_k = 0 \quad (1.1)$$

with the skew-symmetric $2n \times 2n$ matrix $\mathcal{J} := \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$ and the superscript $*$ denoting the conjugate transpose. Here k belongs to a discrete interval $\mathcal{I}_{\mathbb{Z}}$, which is finite or unbounded from above. The conditions in (1.1) imply that $\mathbb{S}_k(\lambda)$ satisfies the following symplectic-type identity

$$\mathbb{S}_k^*(\bar{\lambda}) \mathcal{J} \mathbb{S}_k(\lambda) = \mathcal{J}, \quad (1.2)$$

which motivates the basic terminology for system (\mathbf{S}_λ) . Moreover, system (\mathbf{S}_λ) can be written as

$$\mathcal{J} [z_k(\lambda) - \mathcal{S}_k z_{k+1}(\lambda)] = \lambda \Psi_k z_k(\lambda), \quad \Psi_k := \mathcal{J} \mathcal{S}_k \mathcal{J} \mathcal{V}_k^* \mathcal{J}, \quad (1.3)$$

which gives to rise a linear map \mathcal{L} defined by the left-hand side of (1.3). Note that Ψ also plays the role of the weight matrix in the associated semi-inner product (see Theorem 2.2). Hence, we assume, in addition to (1.1), that Ψ_k is positive semidefinite on $\mathcal{I}_{\mathbb{Z}}$.

System (\mathbf{S}_λ) is said to be in the “time reversed” form. Identity (1.2) implies that the matrix $\tilde{\mathbb{S}}_k(\lambda) := \mathbb{S}_k^{-1}(\lambda) = -\mathcal{J} \mathbb{S}_k^*(\bar{\lambda}) \mathcal{J}$ exists for all $\lambda \in \mathbb{C}$ and $k \in \mathcal{I}_{\mathbb{Z}}$, depends linearly on λ , and satisfies the same equality as in (1.2). Hence system (\mathbf{S}_λ) is equivalent with the (classical and more natural) “forward” discrete symplectic system

$$z_{k+1}(\lambda) = \tilde{\mathbb{S}}_k(\lambda) z_k(\lambda), \quad \tilde{\mathbb{S}}_k(\lambda) := \tilde{\mathcal{S}}_k + \lambda \tilde{\mathcal{V}}_k, \quad (\tilde{\mathbf{S}}_\lambda)$$

i.e., $z(\lambda)$ solves (\mathbf{S}_λ) if and only if it solves system $(\tilde{\mathbf{S}}_\lambda)$. Moreover, the Ψ -norm of a solution $z(\lambda)$ agrees with its $\tilde{\Psi}$ -norm, where $\tilde{\Psi}_k$ denotes the weight matrix corresponding to system $(\tilde{\mathbf{S}}_\lambda)$ and $\tilde{\Psi}_k \geq 0$ if and only if $\Psi_k \geq 0$. This equivalence guarantees that the results of the Weyl–Titchmarsh theory for system $(\tilde{\mathbf{S}}_\lambda)$ established in [6, 9, 37] (see also [39, Section 4]) are also true for system (\mathbf{S}_λ) .

Let us emphasize that analogously we could deal with system $(\tilde{\mathbf{S}}_\lambda)$ instead of (\mathbf{S}_λ) . But the choice of system (\mathbf{S}_λ) is mainly motivated by the absence of the shift on the right-hand side of equality (1.3) and in the associated semi-inner product, which produces more natural calculations, see [10]. This is also the traditional approach in connection with the second order Sturm–Liouville difference equations (see, e.g. [24, 33]). On the other hand, systems (\mathbf{S}_λ) and $(\tilde{\mathbf{S}}_\lambda)$ lead to different spaces of square summable sequences defined in (2.9).

Since the mapping associated with system (\mathbf{S}_λ) may be multivalued or non-densely defined, the approach dealing with linear relations instead of operators is utilized; see [10, Section 5]. The study of linear relations associated with system (\mathbf{S}_λ) begun in [10] is continued in this paper with a characterization of self-adjoint extensions of symmetric linear relations. The description of self-adjoint extensions and their particular cases is a classic problem in the theory of differential and difference equations; see [3, 7, 13, 16, 17, 19, 20, 23, 25, 27–30, 33, 34, 41–44]. As in [31, 42–44] our main result here is obtained by using square summable solutions of system (\mathbf{S}_λ) and the Glazman–Krein–Naimark theory.

In [31], a characterization of self-adjoint extensions is given for linear Hamiltonian difference systems of the form

$$\Delta \begin{pmatrix} x_k(\lambda) \\ u_k(\lambda) \end{pmatrix} = (H_k + \lambda W_k) \begin{pmatrix} x_{k+1}(\lambda) \\ u_k(\lambda) \end{pmatrix}, \quad H_k := \begin{pmatrix} A_k & B_k \\ C_k & -A_k^* \end{pmatrix}, \quad W_k := \begin{pmatrix} 0 & W_k^{[2]} \\ -W_k^{[1]} & 0 \end{pmatrix}, \quad (1.4)$$

where $B_k, C_k, W_k^{[1]}, W_k^{[2]}$ are $n \times n$ Hermitian matrices, $W_k^{[1]} \geq 0, W_k^{[2]} \geq 0$, and the matrix $I - A_k$ is invertible. We note that the underlying discrete interval considered in the latter reference can be also unbounded from below. An interesting overlap exists between the systems given in (S_λ) and (1.4). System (S_λ) can be written as a linear Hamiltonian difference system only if the $n \times n$ matrix in the right-lower block of $\mathbb{S}_k(\lambda)$ is invertible for all $\lambda \in \mathbb{C}$ and $k \in \mathcal{I}_\mathbb{Z}$. However, in this instance the dependence on λ may be nonlinear and the form of W_k more general than in (1.4). On the other hand, system (1.4) can be written as (S_λ) only if $W_k^{[2]}(I - A_k^*)^{-1}W_k^{[1]} \equiv 0$. Without this additional assumption we obtain a discrete symplectic system with a special quadratic dependence on λ , see also [36, 38] for more details.

If we suppress the dependence on the spectral parameter, discrete symplectic systems, i.e., (S_λ) or (\tilde{S}_λ) with $\lambda = 0$, represent the proper discrete counterpart of the linear Hamiltonian differential system (see, e.g. [5]). Hence system (S_λ) can be seen as a discrete analogue of the system

$$z'(t, \lambda) = \mathcal{J}[B(t) + \lambda A(t)] z(t, \lambda), \quad (1.5)$$

where $A(t), B(t)$ are $2n \times 2n$ locally integrable, Hermitian matrix-valued functions (see Remark 2.3). But we point out the principal difference in the assumptions concerning the invertibility of the weight matrices Ψ_k and $A(t)$. Hence we refer to [38], where a connection between linear Hamiltonian differential and difference systems and discrete symplectic systems depending on the spectral parameter is discussed with using the time scale calculus, which provides suitable tools for this purpose.

The rest of the paper is organized as follows: In Section 2, we list notation used, introduce system (S_λ) precisely, and recall several results from the theory of linear relations. We also establish a limit point criterion for system (S_λ) in Theorem 2.7. In Section 3 we present the main result, Theorem 3.3, concerning the characterization of self-adjoint extensions of the minimal linear relation associated with system (S_λ) . We apply this to a consideration of the 2×2 (scalar) case for a finite discrete interval, and describe the Krein–von Neumann extension explicitly: see Theorems 3.9 and 3.11, and Example 3.10. We note that there is no analogue of Theorems 2.7, 3.9, 3.11 and Example 3.10 in the setting of system (1.4). Finally, Section 4 is devoted to the proof of Theorem 3.3.

2. PRELIMINARIES

In the first part of this section we establish the basic notation. The real and imaginary parts of any $\lambda \in \mathbb{C}$ are, respectively, denoted by $\operatorname{Re}(\lambda)$ and $\operatorname{Im}(\lambda)$, i.e., $\operatorname{Re}(\lambda) := (\lambda + \bar{\lambda})/2$ and $\operatorname{Im}(\lambda) := (\lambda - \bar{\lambda})/(2i)$. The symbols \mathbb{C}_+ and \mathbb{C}_- mean, respectively, the upper and lower complex plane, i.e., $\mathbb{C}_+ := \{\lambda \in \mathbb{C} \mid \operatorname{Im}(\lambda) > 0\}$ and $\mathbb{C}_- := \{\lambda \in \mathbb{C} \mid \operatorname{Im}(\lambda) < 0\}$.

All matrices are considered over the field of complex numbers \mathbb{C} . For $r, s \in \mathbb{N}$ we denote by $\mathbb{C}^{r \times s}$ the space of all complex-valued $r \times s$ matrices and $\mathbb{C}^{r \times 1}$ will be abbreviated as \mathbb{C}^r . For a given matrix $M \in \mathbb{C}^{r \times s}$ we indicate by $M^\top, \overline{M}, M^*, \det M, \operatorname{rank} M, M \geq 0, \operatorname{adj}(M), \mathcal{R}(M)$, and $\dim \mathcal{R}(M)$, respectively, its transpose, conjugate, conjugate transpose, determinant, rank, positive definiteness, adjugate matrix, range (i.e., the space spanned by the columns of M) and the dimension of $\mathcal{R}(M)$. By $\|M\|_2$, we denote the spectral norm for $M \in \mathbb{C}^{n \times n}$, i.e., $\|M\|_2 := \max\{\sqrt{\mu} \mid \mu \text{ is an eigenvalue of } M^*M\}$. This norm possesses the submultiplicative property, i.e., $\|MN\|_2 \leq \|M\|_2\|N\|_2$ for any $M, N \in \mathbb{C}^{n \times n}$,

and is the operator norm induced by the Euclidean norm on \mathbb{C}^n , i.e., $\|v\|_2 = (v^*v)^{1/2}$ for any $v \in \mathbb{C}^n$. Hence, we also have

$$\|Mv\|_2 \leq \|M\|_2 \|v\|_2 \quad (2.1)$$

for any $M \in \mathbb{C}^{n \times n}$ and $v \in \mathbb{C}^n$.

In addition, by $M_{u,v}$ we mean the submatrix of $M \in \mathbb{C}^{r \times s}$ consisting of the first $u \leq r$ rows and of the first $v \leq s$ columns and we write only M_u in the case $u = v$, i.e., for the u -th leading principal submatrix of M . The following relations are well known for any matrices $M \in \mathbb{C}^{r \times s}$, $L \in \mathbb{C}^{s \times p}$, and $Q \in \mathbb{C}^{r \times q}$,

$$\text{rank } M + \text{rank } L - s \leq \text{rank } ML \leq \min\{\text{rank } M, \text{rank } L\}, \quad (2.2)$$

$$\text{rank } M = \text{rank } MM^* = \text{rank } M^*M, \quad (2.3)$$

$$\text{rank}(M, Q) + \dim[\mathcal{R}(M) \cap \mathcal{R}(Q)] = \text{rank } M + \text{rank } Q; \quad (2.4)$$

e.g. [4, Corollaries 2.5.1, 2.5.3, and 2.5.10 and Fact 2.11.9].

Let \mathcal{I} be an open or closed interval in \mathbb{R} . Then, $\mathcal{I}_{\mathbb{Z}} := \mathcal{I} \cap \mathbb{Z}$ denotes the corresponding discrete interval. In particular, with $N \in \mathbb{N} \cup \{0, \infty\}$, we shall be interested in discrete intervals of the form $\mathcal{I}_{\mathbb{Z}} := [0, N+1]_{\mathbb{Z}}$, in which case we define $\mathcal{I}_{\mathbb{Z}}^+ := [0, N+1]_{\mathbb{Z}}$ with the understanding that $\mathcal{I}_{\mathbb{Z}} \equiv \mathcal{I}_{\mathbb{Z}}^+$ when $N = \infty$. Hence our system (S_{λ}) will be considered on discrete intervals $\mathcal{I}_{\mathbb{Z}}$ which are finite or unbounded above.

By $\mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{r \times s}$ we denote the space of sequences defined on $\mathcal{I}_{\mathbb{Z}}$ of complex $r \times s$ matrices, where typically $r \in \{n, 2n\}$ and $1 \leq s \leq 2n$. In particular, we write only $\mathbb{C}(\mathcal{I}_{\mathbb{Z}})^r$ in the case $s = 1$. If $M \in \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{r \times s}$, then $M(k) := M_k$ for $k \in \mathcal{I}_{\mathbb{Z}}$ and if $M(\lambda) \in \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{r \times s}$, then $M(\lambda, k) := M_k(\lambda)$ for $k \in \mathcal{I}_{\mathbb{Z}}$ with $M_k^*(\lambda) := [M_k(\lambda)]^*$. If $M \in \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{r \times s}$ and $L \in \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{s \times p}$, then $MN \in \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{r \times p}$, where $(MN)_k := M_k N_k$ for $k \in \mathcal{I}_{\mathbb{Z}}$. The subspace of $\mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{r \times s}$ consisting of all sequences compactly supported in $\mathcal{I}_{\mathbb{Z}}$ is denoted by $\mathbb{C}_0(\mathcal{I}_{\mathbb{Z}})^{r \times s}$. The forward difference operator acting on $\mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{r \times s}$ is denoted by Δ where $(\Delta z)_k := \Delta z_k$. Finally, $z_k|_m^n := z_n - z_m$.

2.1. Discrete symplectic systems. In the previous section system (S_{λ}) was introduced through the matrices \mathcal{S}, \mathcal{V} satisfying (1.1) and such that Ψ given in (1.3) is positive semidefinite. But according to (1.3), system (S_{λ}) can be determined also by \mathcal{S} and a suitable matrix Ψ . This correspondence was shown in [10, Subsection 2.1] and it justifies the following hypothesis concerning the basic conditions for the coefficients of system (S_{λ}) . It guarantees that all the conditions in (1.1) are satisfied, which implies that any initial value problem associated with (S_{λ}) is uniquely solvable on $\mathcal{I}_{\mathbb{Z}}$ for any initial value given at any $k_0 \in \mathcal{I}_{\mathbb{Z}}^+$. This hypothesis is assumed throughout the paper.

Hypothesis 2.1. Let $n \in \mathbb{N}$ and $\mathcal{I}_{\mathbb{Z}}$ be given. We have $\mathcal{S}, \Psi \in \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{2n \times 2n}$ such that

$$\mathcal{S}_k^* \mathcal{J} \mathcal{S}_k = \mathcal{J}, \quad \Psi_k^* = \Psi_k, \quad \Psi_k^* \mathcal{J} \Psi_k = 0, \quad \Psi_k \geq 0 \quad \text{for all } k \in \mathcal{I}_{\mathbb{Z}}. \quad (2.5)$$

Moreover, we define $\mathbb{S}_k(\lambda) := \mathcal{S}_k + \lambda \mathcal{V}_k$ with $\mathcal{V}_k := -\mathcal{J} \Psi_k \mathcal{S}_k$ for all $k \in \mathcal{I}_{\mathbb{Z}}$.

Let us define the linear map

$$\mathcal{L} : \mathbb{C}(\mathcal{I}_{\mathbb{Z}}^+)^{2n} \rightarrow \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{2n}, \quad \mathcal{L}(z)_k := \mathcal{J}(z_k - \mathcal{S}_k z_{k+1}).$$

Then the nonhomogeneous problem

$$z_k(\lambda) = \mathbb{S}_k(\lambda) z_{k+1}(\lambda) - \mathcal{J} \Psi_k f_k, \quad k \in \mathcal{I}_{\mathbb{Z}}, \quad (S_{\lambda}^f)$$

where $f \in \mathbb{C}(\mathcal{I}_{\mathbb{Z}})^{2n}$, can be written as

$$\mathcal{L}(z(\lambda))_k = \lambda \Psi_k z_k(\lambda) + \Psi_k f_k, \quad k \in \mathcal{I}_{\mathbb{Z}};$$

see [10, Lemma 2.6]. For convenience, we abbreviate $\mathcal{L}^*(z)_k := [\mathcal{L}(z)_k]^*$ and by (S_ν^g) we will refer to the nonhomogeneous system of the form (S_λ^f) with λ replaced by ν and f replaced by g . Analogous notation is employed also for system (S_λ) , which corresponds to (S_λ^0) . We also suppress the dependence of $z(\lambda)$ on λ when $\lambda = 0$.

The following identity is crucial in the whole theory (see [10, Theorem 2.5] for its proof).

Theorem 2.2 (Extended Lagrange identity). *Let $\lambda, \nu \in \mathbb{C}$, $1 \leq m \leq 2n$, and $f, g \in \mathbb{C}(\mathcal{I}_\mathbb{Z})^{2n \times m}$. If $z(\lambda) \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n \times m}$ and $u(\nu) \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n \times m}$ are solutions of systems (S_λ^f) and (S_ν^g) , respectively, then for any $k, s, t \in \mathcal{I}_\mathbb{Z}$ such that $s \leq t$, we have*

$$\begin{aligned} \Delta[z_k^*(\lambda) \mathcal{J} u_k(\nu)] &= (\bar{\lambda} - \nu) z_k^*(\lambda) \Psi_k u_k(\nu) + f_k^* \Psi_k u_k(\nu) - z_k^*(\lambda) \Psi_k g_k, \\ z_k^*(\lambda) \mathcal{J} u_k(\nu) \Big|_s^{t+1} &= \sum_{k=s}^t \{ (\bar{\lambda} - \nu) z_k^*(\lambda) \Psi_k u_k(\nu) + f_k^* \Psi_k u_k(\nu) - z_k^*(\lambda) \Psi_k g_k \}. \end{aligned} \quad (2.6)$$

Epecially, if $\nu = \bar{\lambda}$ and $f \equiv 0 \equiv g$, we get the Wronskian-type identity

$$z_k^*(\lambda) \mathcal{J} u_k(\bar{\lambda}) = z_0^*(\lambda) \mathcal{J} u_0(\bar{\lambda}), \quad k \in \mathcal{I}_\mathbb{Z}^+. \quad (2.7)$$

Since we assume $\Psi_k \geq 0$ on $\mathcal{I}_\mathbb{Z}$, Theorem 2.2 motivates the natural definition of the semi-inner product for $z, u \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n}$ as

$$\langle z, u \rangle_\Psi := \sum_{k \in \mathcal{I}_\mathbb{Z}} z_k^* \Psi_k u_k \quad (2.8)$$

and of the semi-norm $\|z\|_\Psi := \sqrt{\langle z, z \rangle_\Psi}$. Then we denote by ℓ_Ψ^2 the linear space of all square summable sequences defined on $\mathcal{I}_\mathbb{Z}^+$, i.e.,

$$\ell_\Psi^2 = \ell_\Psi^2(\mathcal{I}_\mathbb{Z}) := \{z \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n} \mid \|z\|_\Psi < \infty\}. \quad (2.9)$$

Identity (2.6) can be written as

$$(z(\lambda), u(\nu))_k \Big|_s^{t+1} = \sum_{k=s}^t \{ \mathcal{L}^*(z(\lambda))_k u_k(\nu) - z_k^*(\lambda) \mathcal{L}(u(\nu))_k \}, \quad (2.10)$$

where we use for any $z, u \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n}$ and $k \in \mathcal{I}_\mathbb{Z}^+$ the notation

$$(z, u)_k := z_k^* \mathcal{J} u_k.$$

Moreover, under the assumptions of Theorem 2.2 with $\lambda = 0 = \nu$, $m = 1$, $s = 0$, and $t = N$ we get from (2.6) and (2.8) that

$$(z, u)_k \Big|_0^{N+1} = \langle f, u \rangle_\Psi - \langle z, g \rangle_\Psi, \quad (2.11)$$

where the left-hand side of (2.11) means $\lim_{k \rightarrow \infty} (z, u)_k - (z, u)_0$ if $\mathcal{I}_\mathbb{Z} = [0, \infty)_\mathbb{Z}$. Identity (2.11) shows that the latter limit exists finite whenever $z, u, f, g \in \ell_\Psi^2$.

Remark 2.3. Similarly as in the continuous case, there exists a unitary map $Q : \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n} \rightarrow \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n}$ preserving the square summability with respect to Ψ and such that system (S_0^f) can be written in the canonical form, i.e., with $\mathcal{S} \equiv I$. Indeed, let Φ denote the fundamental matrix of system (S_0^0) satisfying $\Phi_0 = I$. Then, it is invertible for all $k \in \mathcal{I}_\mathbb{Z}^+$ with $\Phi_k^{-1} = -\mathcal{J} \Phi_k^* \mathcal{J}$ and this inverse provides the canonical transformation, i.e., $Q = \Phi^{-1}$ with $Q(z)_k := \Phi_k^{-1} z_k$. Hence system (S_0^f) is equivalent with

$$-\mathcal{J} \Delta y_k = \widehat{\Psi}_k g_k, \quad k \in \mathcal{I}_\mathbb{Z}, \quad (2.12)$$

where $y_k := Q(z)_k$, $g_k := Q(f)_k$, and $\widehat{\Psi}_k := \Phi_k^* \Psi_k \Phi_k$. One can easily verify that $y \in \ell_{\widehat{\Psi}}^2$ if and only if $z \in \ell_{\Psi}^2$. System (2.12) can be seen as a discrete counterpart of the canonical linear Hamiltonian differential system, i.e., nonhomogeneous system associated with (1.5), where $B(t) \equiv 0$; e.g. [26, Subsection 2.2] and the references therein.

It is known that some Atkinson-type (or definiteness) condition is needed for the study of square summable solutions of discrete symplectic systems, see [10, 37]. These conditions guarantee that some (the “weak” condition) or all (the “strong” condition) nontrivial solutions $z(\lambda)$ of (S_λ) satisfy $\|z(\lambda)\|_\Psi \neq 0$. The precise distinguishing between the weak and strong formulation of the Atkinson-type condition enables one to formulate some results of the Weyl–Titchmarsh theory for discrete symplectic systems with coupled (or jointly varying) endpoints, see [35]. On the other hand, the strong condition implies the equality between the number of linearly independent square summable solutions of system (S_λ) and the deficiency index corresponding to the minimal linear relation associated with (S_λ) , see [10, Corollary 5.12]. Since this relation shall be necessary for our treatment, we need the following hypothesis, see [10, Section 3].

Hypothesis 2.4 (Strong Atkinson condition). There exists a finite interval $\mathcal{I}_\mathbb{Z}^\mathbb{D} := [a, b]_\mathbb{Z} \subseteq \mathcal{I}_\mathbb{Z}$ such that for any $\lambda \in \mathbb{C}$ every nontrivial solution $z(\lambda) \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n}$ of system (S_λ) satisfies

$$\sum_{k=a}^b z_k^*(\lambda) \Psi_k z_k(\lambda) > 0.$$

The positive semidefiniteness of Ψ and Hypothesis 2.4 imply that

$$0 < \sum_{k=a}^b z_k^*(\lambda) \Psi_k z_k(\lambda) \leq \sum_{k \in \widetilde{\mathcal{I}}_\mathbb{Z}} z_k^*(\lambda) \Psi_k z_k(\lambda) \quad (2.13)$$

for any discrete interval $\widetilde{\mathcal{I}}_\mathbb{Z}$ such that $\mathcal{I}_\mathbb{Z}^\mathbb{D} \subseteq \widetilde{\mathcal{I}}_\mathbb{Z} \subseteq \mathcal{I}_\mathbb{Z}$.

Example 2.5.

- (i) As demonstrated in [10, Example 3.4], the simplest example of system (S_λ) satisfying Hypothesis 2.4 is represented by the scalar system

$$\begin{pmatrix} x_k(\lambda) \\ u_k(\lambda) \end{pmatrix} = \begin{pmatrix} 1 & -1/p_{k+1} \\ -q_k + \lambda w_k & 1 + (q_k - \lambda w_k)/p_{k+1} \end{pmatrix} \begin{pmatrix} x_{k+1}(\lambda) \\ u_{k+1}(\lambda) \end{pmatrix}, \quad k \in \mathcal{I}_\mathbb{Z}, \quad (2.14)$$

where p_k, q_k, w_k are real-valued and such that $p_k \neq 0$ on $\mathcal{I}_\mathbb{Z}^+$, q_k is defined on $\mathcal{I}_\mathbb{Z}$, $w_k \geq 0$ on $\mathcal{I}_\mathbb{Z}$, and $w_k > 0$ at least at two consecutive points of $\mathcal{I}_\mathbb{Z}$. In this case $\Psi_k = \begin{pmatrix} w_k & 0 \\ 0 & 0 \end{pmatrix}$. System (2.14) includes the second order Sturm–Liouville difference equation

$$-\Delta[p_k \Delta y_{k-1}(\lambda)] + q_k y_k(\lambda) = \lambda w_k y_k(\lambda), \quad k \in \mathcal{I}_\mathbb{Z}, \quad (2.15)$$

(put $x_k = y_k$ and $u_k = p_k \Delta y_{k-1}$). Note that a solution $y(\lambda)$ of the latter equation is defined on the discrete interval $\{-1\} \cup \mathcal{I}_\mathbb{Z}^+$.

- (ii) System (2.14) is a particular case of system (S_λ) with the special linear dependence on λ , i.e.,

$$(S_\lambda), \quad \mathcal{S}_k = \begin{pmatrix} \mathcal{A}_k & \mathcal{B}_k \\ \mathcal{C}_k & \mathcal{D}_k \end{pmatrix}, \quad \mathcal{V}_k = \begin{pmatrix} 0 & 0 \\ \mathcal{W}_k \mathcal{A}_k & \mathcal{W}_k \mathcal{B}_k \end{pmatrix}, \quad k \in \mathcal{I}_\mathbb{Z}, \quad (2.16)$$

where the $n \times n$ blocks are such that \mathcal{S}_k satisfies the first equality in (2.5) and $\mathcal{W}_k = \mathcal{W}_k^* \geq 0$. Then Hypothesis 2.1 holds with $\Psi_k = \begin{pmatrix} \mathcal{W}_k & 0 \\ 0 & 0 \end{pmatrix}$, because the first equality in (2.5) equivalent with

(suppressing the argument $k \in \mathcal{I}_\mathbb{Z}$)

$$\mathcal{A}^* \mathcal{D} - \mathcal{C}^* \mathcal{B} = I = \mathcal{A} \mathcal{D}^* - \mathcal{B} \mathcal{C}^* \quad \text{and} \quad \mathcal{A}^* \mathcal{C}, \mathcal{B}^* \mathcal{D}, \mathcal{A} \mathcal{B}^*, \mathcal{C} \mathcal{D}^* \text{ are Hermitian.} \quad (2.17)$$

In addition, if there exists an index $l \in \mathcal{I}_\mathbb{Z} \setminus \{0\}$ such that the matrices $\mathcal{B}_{l-1}, \mathcal{W}_{l-1}, \mathcal{W}_l$ are invertible, then also Hypothesis 2.4 is satisfied, see [10, Theorem 3.11].

▲

Remark 2.6. If $q(\lambda)$ denotes the number of linearly independent square summable solution of system (S_λ) for $\lambda \in \mathbb{C}$, i.e.,

$$q(\lambda) := \dim Q(\lambda), \quad Q(\lambda) := \{z \in \ell_\Psi^2 \mid z(\lambda) \text{ solves } (S_\lambda)\}, \quad (2.18)$$

then under Hypothesis 2.4 (even its “weak” form) we have $n \leq q(\lambda) \leq 2n$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$, see [37, Section 4] for more details. The geometrical background of this estimate leads to the classification of system (S_λ) as being in the limit point case if $q(\lambda) = n$, and as being in the limit circle case if $q(\lambda) = 2n$. Moreover, if there exists $\lambda_0 \in \mathbb{C}$ such that $q(\lambda_0) = 2n$, then $q(\lambda) \equiv 2n$ on \mathbb{C} , whether Hypothesis 2.4 is satisfied or not, see [37, Theorem 4.17] and compare with the results in [39]. The latter statement is known as the invariance of the limit circle case and a sufficient condition for this situation can be found in [37, Corollary 4.18]. Consequently, under Hypothesis 2.4 (even its weak form) and with $n = 1$, we obtain the generalization of the well-known Weyl alternative: either all solutions of (S_λ) belong to ℓ_Ψ^2 for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$, or there exists only one nontrivial solution in ℓ_Ψ^2 for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$ (see [37, Corollary 4.19]). Sufficient conditions for the invariance of $q(\lambda)$ in the case $q(\lambda_0) < 2n$ remain open.

The classical limit point criterion for linear Hamiltonian differential and difference systems (1.4) and (1.5) utilizes the minimal eigenvalue of the corresponding weight matrix. Unfortunately, similar criterion cannot be applied in the current setting, because the weight matrix Ψ_k is always singular, see also [37, Remark 4.16]. In the following theorem we give conditions guaranteeing the invariance of the limit point case on $\mathbb{C} \setminus \mathbb{R}$ for system (S_λ) with the special linear dependence on λ as discussed in Example 2.5(ii). This statement is a discrete analogue of [26, Theorem 5.6].

Theorem 2.7. Let $\mathcal{I}_\mathbb{Z} = [0, \infty)_\mathbb{Z}$ and consider system (2.16) such that $\mathcal{B}_k^* \mathcal{C}_k \equiv 0$, $\mathcal{B}_k^* \mathcal{D}_k > 0$, and $\mathcal{W}_k > 0$ for all $k \in \mathcal{I}_\mathbb{Z}$. If there exists $h \in \mathbb{C}(\mathcal{I}_\mathbb{Z})^1$ such that $h_k \geq h > 0$ and

$$\mathcal{A}_k^* \mathcal{C}_k \geq -h_k \mathcal{W}_{k+1}, \quad \sum_{k=0}^{\infty} \frac{1}{g_k \sqrt{h_k}} = \infty, \quad (2.19)$$

where $g_k := \max \{1, \|\mathcal{W}_{k+1}^{-1/2} (\mathcal{B}_k^* \mathcal{D}_k)^{-1/2}\|_2\}$, and a constant $T \geq 0$ such that

$$\Delta\left(\frac{1}{h_k}\right) g_k \leq \frac{T}{\sqrt{h_k}}, \quad k \in \mathcal{I}_\mathbb{Z}, \quad (2.20)$$

then system (S_λ) is in the limit point case for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$, i.e., $q(\lambda) = n$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

Proof. The special structure of the coefficient matrices implies that system (S_λ) can be written as

$$\begin{aligned} x_k &= \mathcal{A}_k x_{k+1} + \mathcal{B}_k u_{k+1}, \\ u_k &= (\mathcal{C}_k + \lambda \mathcal{W}_k \mathcal{A}_k) x_{k+1} + (\mathcal{B}_k + \lambda \mathcal{W}_k \mathcal{B}_k) u_{k+1} = \mathcal{C}_k x_{k+1} + \mathcal{B}_k u_{k+1} + \lambda \mathcal{W}_k x_k, \end{aligned}$$

with $\Psi_k = \begin{pmatrix} \mathcal{W}_k & 0 \\ 0 & 0 \end{pmatrix}$. The invertibility of \mathcal{B}_k and \mathcal{W}_k for all $k \in \mathcal{I}_\mathbb{Z}$ implies that Hypothesis 2.4 holds, see [10, Theorem 3.11]. In accordance with [37, Theorem 4.4], and with $q(\lambda)$ defined in (2.18), we have $q(\lambda) = n$ if and only if $\tilde{Z}_k(\lambda)\beta \notin \ell_\Psi^2$ for any $\beta \in \mathbb{C}^n \setminus \{0\}$, where $\tilde{Z}(\lambda)$ is the $2n \times n$ solution

of system (S_λ) determined by the initial condition $\tilde{Z}_0(\lambda) = -\mathcal{J}\alpha^*$ with $\alpha \in \mathbb{C}^{n \times 2n}$ being such that $\alpha \alpha^* = I$ and $\alpha \mathcal{J} \alpha^* = 0$. Moreover, it is sufficient to consider only $\lambda = \pm i$, because the number $q(\lambda) \geq n$ is constant in \mathbb{C}_+ and \mathbb{C}_- by [10, Corollary 5.12]. Hence, let $\beta \in \mathbb{C}^n \setminus \{0\}$ and $\lambda \in \{\pm i\}$ be fixed. Let us denote $z_k := \begin{pmatrix} x_k \\ u_k \end{pmatrix} = \tilde{Z}_k(\lambda) \beta$ with the $n \times 1$ components x_k, u_k and $k \in \mathcal{I}_\mathbb{Z}$. Note that $z_0^* \mathcal{J} z_0 = 0$. We show that under the current assumptions we have $z \notin \ell_\Psi^2$.

Let us assume that $z \in \ell_\Psi^2$. By a direct calculation, we obtain from the block structure of the system and the identities in (2.17) that

$$\Delta(x_k^* u_k) = -x_{k+1}^* \mathcal{A}_k^* \mathcal{C}_k x_{k+1} - x_{k+1}^* \mathcal{C}_k^* \mathcal{B}_k u_{k+1} - u_{k+1}^* \mathcal{B}_k^* \mathcal{C}_k x_{k+1} - u_{k+1}^* \mathcal{B}_k^* \mathcal{D}_k u_{k+1} - \lambda x_k^* \mathcal{W}_k x_k.$$

Since $\mathcal{B}_k^* \mathcal{D}_k > 0$ and $h_k > 0$, the quantity $\mathcal{F}_k(x, u) := \left(\sum_{j=0}^k \frac{1}{h_j} u_{j+1}^* \mathcal{B}_j^* \mathcal{D}_j u_{j+1} \right)^{1/2} \geq 0$ is well-defined. Then the latter equality and the assumption $\mathcal{B}_k^* \mathcal{C}_k \equiv 0$ yield

$$\mathcal{F}_k^2(x, u) = - \sum_{j=0}^k \frac{1}{h_j} x_{j+1}^* \mathcal{A}_j^* \mathcal{C}_j x_{j+1} - \lambda \sum_{j=0}^k \frac{1}{h_j} x_j^* \mathcal{W}_j x_j - \sum_{j=0}^k \frac{1}{h_j} \Delta(x_j^* u_j). \quad (2.21)$$

From the Hermitian property and positive definiteness of \mathcal{W}_k and $\mathcal{B}_k^* \mathcal{D}_k$, the Cauchy–Schwarz inequality, inequality (2.1), and the definition of g_k we obtain

$$\begin{aligned} |x_{k+1}^* u_{k+1}| &= |(\mathcal{W}_{k+1}^{1/2} x_{k+1})^* \mathcal{W}_{k+1}^{-1/2} (\mathcal{B}_k^* \mathcal{D}_k)^{-1/2} (\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}| \\ &\leq \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2 \times \|\mathcal{W}_{k+1}^{-1/2} (\mathcal{B}_k^* \mathcal{D}_k)^{-1/2} (\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2 \\ &\leq \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2 \times \|\mathcal{W}_{k+1}^{-1/2} (\mathcal{B}_k^* \mathcal{D}_k)^{-1/2}\|_2 \times \|(\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2 \\ &\leq g_k \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2 \times \|(\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2. \end{aligned} \quad (2.22)$$

Hence the latter inequality, assumption (2.20), the Cauchy–Schwarz inequality, and the inequality of arithmetic and geometric means $\sqrt{ab} \leq \frac{a+b}{2}$ yield

$$\begin{aligned} \left| \sum_{j=0}^k \Delta\left(\frac{1}{h_j}\right) x_{j+1}^* u_{j+1} \right| &\leq \sum_{j=0}^k \Delta\left(\frac{1}{h_j}\right) |x_{j+1}^* u_{j+1}| \leq \sum_{j=0}^k \Delta\left(\frac{1}{h_j}\right) g_j \|\mathcal{W}_{j+1}^{1/2} x_{j+1}\|_2 \times \|(\mathcal{B}_j^* \mathcal{D}_j)^{1/2} u_{j+1}\|_2 \\ &\leq \sum_{j=0}^k T \|\mathcal{W}_{j+1}^{1/2} x_{j+1}\|_2 \times h_j^{-1/2} \|(\mathcal{B}_j^* \mathcal{D}_j)^{1/2} u_{j+1}\|_2 \\ &\leq \left(T^2 \sum_{j=0}^k \|\mathcal{W}_{j+1}^{1/2} x_{j+1}\|_2^2 \right)^{1/2} \times \left(\sum_{j=0}^k h_j^{-1} \|(\mathcal{B}_j^* \mathcal{D}_j)^{1/2} u_{j+1}\|_2^2 \right)^{1/2} \\ &\leq \frac{1}{2} \left(T^2 \sum_{j=0}^k \|\mathcal{W}_{j+1}^{1/2} x_{j+1}\|_2^2 + \sum_{j=0}^k h_j^{-1} \|(\mathcal{B}_j^* \mathcal{D}_j)^{1/2} u_{j+1}\|_2^2 \right) \\ &\leq \frac{1}{2} (T^2 \|z\|_\Psi^2 + \mathcal{F}_k^2(x, u)). \end{aligned} \quad (2.23)$$

By using the summation by parts together with the inequalities $h_k \geq h$, (2.22), and (2.23) we get

$$\begin{aligned} \left| \operatorname{Re} \sum_{j=0}^k \frac{1}{h_j} \Delta(x_j^* u_j) \right| &\leq \left| \sum_{j=0}^k \frac{1}{h_j} \Delta(x_j^* u_j) \right| \leq \left| [x_j^* u_j / h_j]_0^{k+1} - \sum_{j=0}^k \Delta\left(\frac{1}{h_j}\right) x_{j+1}^* u_{j+1} \right| \\ &\leq |x_0^* u_0 / h_0| + |x_{k+1}^* u_{k+1} / h_{k+1}| + \left| \sum_{j=0}^k \Delta\left(\frac{1}{h_j}\right) x_{j+1}^* u_{j+1} \right| \\ &\leq T_1 + \frac{1}{h} g_k \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2 \times \|(\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2 + (T^2 \|z\|_\Psi^2 + \mathcal{F}_k^2(x, u))/2, \end{aligned} \quad (2.24)$$

where $T_1 := |x_0^* u_0 / h_0|$. Since $\operatorname{Re}(\mathcal{F}_k^2(x, u)) = -\sum_{j=0}^k \frac{1}{h_j} x_{j+1}^* \mathcal{A}_j^* \mathcal{C}_j x_{j+1} - \operatorname{Re}\left(\sum_{j=0}^k \frac{1}{h_j} \Delta(x_j^* u_j)\right)$ and the inequality in (2.19) implies $-\sum_{j=0}^k \frac{1}{h_j} x_{j+1}^* \mathcal{A}_j^* \mathcal{C}_j x_{j+1} \leq \sum_{j=0}^k x_{j+1}^* \mathcal{W}_j x_{j+1} \leq \|z\|_\Psi^2$, it follows from (2.21) and (2.24) that

$$\frac{1}{2} \sum_{j=0}^k g_j^{-1} h_j^{-1/2} \mathcal{F}_j^2(x, u) \leq T_2 \sum_{j=0}^k g_j^{-1} h_j^{-1/2} + \frac{1}{h} \sum_{j=0}^k h_j^{-1/2} \|\mathcal{W}_{j+1}^{1/2} x_{j+1}\|_2 \times \|(\mathcal{B}_j^* \mathcal{D}_j)^{1/2} u_{j+1}\|_2,$$

where $T_2 := T_1 + (1 + T^2/2) \|z\|_\Psi^2$. Then with the aid of the Cauchy–Schwarz inequality we have

$$\begin{aligned} G_k &:= \frac{1}{2} \sum_{j=0}^k g_j^{-1} h_j^{-1/2} [\mathcal{F}_j^2(x, u) - 2T_2] \leq \frac{1}{h} \left(\sum_{j=0}^k \|\mathcal{W}_{j+1}^{1/2} x_{j+1}\|_2^2 \right)^{1/2} \times \left(\sum_{j=0}^k \|(\mathcal{B}_j^* \mathcal{D}_j)^{1/2} u_{j+1}\|_2^2 \right)^{1/2} \\ &\leq \frac{1}{h} \|z\|_\Psi \mathcal{F}_k(x, u). \end{aligned} \quad (2.25)$$

In the next part we show that $\mathcal{F}_k^2(x, u) \leq 2T_2$ for all $k \in \mathcal{I}_\mathbb{Z}$. Assume that there exists an index $m \in \mathcal{I}_\mathbb{Z}$ such that $\mathcal{F}_m^2(x, u) > 2T_2$. Since $\mathcal{F}_k^2(x, u)$ is nondecreasing, we have $\mathcal{F}_k^2(x, u) - 2T_2 > t$ for all $k \in [m, \infty)_\mathbb{Z}$, where $t := \mathcal{F}_m^2(x, u) - 2T_2$. Also G_k is nondecreasing for all $k \in [m-1, \infty)_\mathbb{Z}$ and for all $k \in [m, \infty)_\mathbb{Z}$ we obtain from (2.25) and the equality $\mathcal{F}_k^2(x, u) = 2g_k h_k^{1/2} \Delta G_{k-1} + 2T_2$ that

$$h^2 - 2\|z\|_\Psi^2 G_k^{-2} T_2 \leq 2G_k^{-2} \|z\|_\Psi^2 g_k h_k^{1/2} \Delta G_{k-1}. \quad (2.26)$$

In addition, $G_k \geq \frac{t}{2} \sum_{j=0}^k g_j^{-1} h_j^{-1/2} \rightarrow \infty$ for $k \rightarrow \infty$ by the second part of (2.19). Now, let $0 < a < 2h^2$ be arbitrary and $l \in [m, \infty)_\mathbb{Z}$ be such that $G_l \geq 2\|z\|_\Psi T_2^{1/2} / \sqrt{2h^2 - a}$. Then we have $a/2 \leq h^2 - 2G_k^{-2} T_2 \|z\|_\Psi^2$ for all $k \in [l, \infty)_\mathbb{Z}$, which together with (2.26) yields for $k \in [l+1, \infty)_\mathbb{Z}$ that

$$\begin{aligned} \frac{a}{2} \sum_{j=l+1}^k \frac{1}{g_j h_j^{1/2}} &\leq \sum_{j=l+1}^k \frac{1}{g_j h_j^{1/2}} (h^2 - 2G_j^{-2} T_2 \|z\|_\Psi^2) \leq \sum_{j=l+1}^k 2G_j^{-2} \|z\|_\Psi^2 \Delta G_{j-1} \\ &\leq 2\|z\|_\Psi^2 \sum_{j=l+1}^k \frac{\Delta G_{j-1}}{G_j G_{j-1}} \leq -2\|z\|_\Psi^2 \sum_{j=l+1}^k \Delta\left(\frac{1}{G_{j-1}}\right) \leq 2\|z\|_\Psi^2 \frac{1}{G_l} < \infty. \end{aligned}$$

But it contradicts the second condition in (2.19) for $k \rightarrow \infty$. Thus $\mathcal{F}_k^2(x, u) \leq 2T_2$ for all $k \in \mathcal{I}_\mathbb{Z}$, i.e.,

$$\sum_{j=0}^{\infty} h_j^{-1} u_{j+1}^* \mathcal{B}_j^* \mathcal{D}_j u_{j+1} \leq 2T_2 < \infty. \quad (2.27)$$

Since system (S_λ) satisfies Hypothesis 2.4, there exists $p \in \mathcal{I}_\mathbb{Z}$ such that $\sum_{j=0}^p z_k^* \Psi_j z_k = T_3 > 0$. Hence the positive definiteness of \mathcal{W}_k and the Lagrange identity in (2.6) yield

$$|z_{k+1}^* \mathcal{J} z_{k+1}| = \left| z_0^* \mathcal{J} z_0 \pm 2i \sum_{j=0}^k z_j^* \Psi_j z_j \right| = 2 \left| \sum_{j=0}^k z_j^* \Psi_j z_j \right| \geq 2 \left| \sum_{j=0}^p z_j^* \Psi_j z_j \right| = 2 T_3, \quad (2.28)$$

for any $k \geq p$. Simultaneously, we get from (2.22) the estimate

$$|z_{k+1}^* \mathcal{J} z_{k+1}| \leq 2 |x_{k+1}^* u_{k+1}| \leq 2 g_k h_k^{1/2} \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2 \times h_j^{-1/2} \|(\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2. \quad (2.29)$$

The inequalities (2.27), (2.28), (2.29), and the Cauchy–Schwarz inequality imply for $k \geq p$ that

$$\begin{aligned} \sum_{j=p}^k \frac{1}{g_j h_j^{1/2}} &\leq \sum_{j=p}^k \frac{2}{|z_{j+1}^* \mathcal{J} z_{j+1}|} \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2 \times h_j^{-1/2} \|(\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2 \\ &\leq \frac{1}{T_3} \sum_{j=p}^k \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2 \times h_j^{-1/2} \|(\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2 \\ &\leq \frac{1}{T_3} \left(\sum_{j=p}^k \|\mathcal{W}_{k+1}^{1/2} x_{k+1}\|_2^2 \right)^{1/2} \times \left(\sum_{j=p}^k h_j^{-1} \|(\mathcal{B}_k^* \mathcal{D}_k)^{1/2} u_{k+1}\|_2^2 \right)^{1/2} \leq \frac{1}{T_3} \|z\|_\Psi \sqrt{2} T_2^{1/2} < \infty, \end{aligned}$$

which (again) contradicts the second condition in (2.19) for $k \rightarrow \infty$. Hence $z \notin \ell_\Psi^2$. Since β and λ were chosen arbitrarily, it follows that $\tilde{Z}(\lambda) \beta \notin \ell_\Psi^2$ for any $\beta \in \mathbb{C}^n \setminus \{0\}$. Therefore, system (S_λ) is in the limit point case for $\lambda \in \{\pm i\}$ and consequently for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$. ■

Upon applying Theorem 2.7 to system (2.14) with $q_k \equiv 0$ we obtain the following corollary for a special case of the second order Sturm–Liouville difference equation (2.15), because one easily observes that $z(\lambda) \in \ell_\Psi^2$ if and only if $\sum_{k=0}^\infty |y_k(\lambda)|^2 w_k < \infty$, where $z_k(\lambda) = (y_k(\lambda), p_k \Delta y_{k-1}(\lambda))^\top$ and $\Psi_k = \begin{pmatrix} w_k & 0 \\ 0 & 0 \end{pmatrix}$.

Corollary 2.8. *Let $\mathcal{I}_\mathbb{Z} = [0, \infty)_\mathbb{Z}$ and consider equation (2.15) with $q_k \equiv 0$, $p_k < 0$ and $w_k > 0$ for all $k \in \mathcal{I}_\mathbb{Z}$. If there exist $h_k \in \mathbb{C}(\mathcal{I}_\mathbb{Z})^1$ and a constant $T \geq 0$ such that $h_k \geq h > 0$ and*

$$\sum_{k=0}^\infty \frac{1}{g_k \sqrt{h_k}} = \infty, \quad \Delta\left(\frac{1}{h_k}\right) g_k \leq \frac{T}{\sqrt{h_k}}, \quad k \in \mathcal{I}_\mathbb{Z}, \quad (2.30)$$

where $g_k := \max\left\{1, \left(-\frac{p_{k+1}}{w_{k+1}}\right)^{1/2}\right\}$, then equation (2.15) is in the limit point case for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$, i.e., there exists only one nontrivial solution satisfying $\sum_{k=0}^\infty |y_k(\lambda)|^2 w_k < \infty$.

It was shown in [24, Theorem 10], see also [40, Corollary 3.1], that equation (2.15) with $p_k \neq 0$ and $w_k > 0$ is in the limit point case for any $\lambda \in \mathbb{C} \setminus \mathbb{R}$ if $\sum_{k=0}^\infty \frac{(w_k w_{k+1})^{1/2}}{|p_{k+1}|} = \infty$. Corollary 2.8 partially generalizes this classical limit-point criterion as shown in the following example.

Example 2.9. Let us consider the equation

$$(2.15), \quad p_k \equiv -1, \quad q_k \equiv 0, \quad w_k = 1/(k+1)^2. \quad (2.31)$$

Then the criterion from [24, Theorem 10] cannot be applied, because

$$\sum_{k=0}^\infty \frac{(w_k w_{k+1})^{1/2}}{|p_{k+1}|} = \sum_{k=0}^\infty \sqrt{\frac{1}{(k+1)^2 (k+2)^2}} = 1 < \infty.$$

On the other hand, the assumptions of Corollary 2.8 are satisfied with $h_k \equiv 1$, $g_k = (k + 2)$, and $T = 0$, i.e., equation (2.31) is in the limit point case for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$. This fact can also be verified by using the Weyl alternative; e.g. [2, Theorem 5.6.1]. Indeed, equation (2.31) with $\lambda = 0$ has two linearly independent solutions $y_k^{[1]} \equiv 1$ and $y_k^{[2]} = k$ for $k \in \{-1\} \cup \mathcal{I}_z$. Since only $y^{[1]}$ is square summable with respect to w_k , it follows from the Weyl alternative that equation (2.31) has to be in the limit point case for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$. \blacktriangle

In the following lemma we establish a basic result concerning the solvability of a boundary value problem associated with (S_λ) , which will be crucial in the proof of Lemma 3.1. It provides the symplectic counterpart of the original Naimark's result known as the "Patching lemma", see [28, Lemma 2 in Section 17.3]. Analogous result for system (1.4) can be found in [31, Lemma 3.3].

Lemma 2.10. *Let Hypothesis 2.4 be satisfied and a finite discrete interval $\tilde{\mathcal{I}}_z := [c, d]_z$ be given such that $\mathcal{I}_z^D \subseteq \tilde{\mathcal{I}}_z \subseteq \mathcal{I}_z$. Then for any given $\alpha, \beta \in \mathbb{C}^{2n}$ there exists $f \in \mathbb{C}(\tilde{\mathcal{I}}_z)^{2n}$ such that the boundary value problem*

$$\mathcal{L}(z)_k = \Psi_k f_k, \quad z_c = \alpha, \quad z_{d+1} = \beta, \quad k \in \tilde{\mathcal{I}}_z, \quad (2.32)$$

has a solution $z \in \mathbb{C}(\tilde{\mathcal{I}}_z^+)^{2n}$, where $\tilde{\mathcal{I}}_z^+ := [c, d + 1]_z$.

Proof. Let A be a $2n \times 2n$ matrix with the elements $a_{ij} := \sum_{k=c}^d \varphi_k^{[i]*} \Psi_k \varphi_k^{[j]}$ for $i, j \in \{1, \dots, 2n\}$, where $\varphi^{[1]}, \dots, \varphi^{[2n]} \in \mathbb{C}(\mathcal{I}_z^+)^{2n}$ are linearly independent solutions of system (S_0) , i.e., $\mathcal{L}(\varphi^{[i]})_k = 0$ for all $k \in \mathcal{I}_z$ and $i \in \{1, \dots, 2n\}$. Then the homogeneous system of algebraic equations $A\xi = 0$, where $\xi = (\xi_1, \dots, \xi_{2n})^\top \in \mathbb{C}^{2n}$, is equivalent with $\sum_{k=c}^d \varphi_k^* \Psi_k \varphi_k = 0$, where $\varphi_k := \sum_{i=1}^{2n} \xi_i \varphi_k^{[i]}$. Since φ also solves system (S_0) , it follows from Hypothesis 2.4 and inequality (2.13) that φ is a trivial solution of (S_0) , i.e., $\sum_{i=1}^{2n} \xi_i \varphi_k^{[i]} \equiv 0$, which implies that $\xi_i = 0$ for all $i \in \{1, \dots, 2n\}$. It yields the invertibility of the matrix A .

Hence there exists a unique solution $\eta = (\eta_1, \dots, \eta_{2n})^\top \in \mathbb{C}^{2n}$ of the nonhomogeneous system of algebraic equations

$$\eta^* A = \beta^* \mathcal{J} \Phi_{d+1}, \quad (2.33)$$

where $\Phi := (\varphi^{[1]*}, \dots, \varphi^{[2n]*})^*$ is a fundamental matrix of (S_0) . If we put $h_k^{[1]} := \Phi_k \eta$ for $k \in \tilde{\mathcal{I}}_z$, we get from (2.33) for all $i \in \{1, \dots, 2n\}$ that

$$\sum_{k=c}^d h_k^{[1]*} \Psi_k \varphi_k^{[i]} = \beta^* \mathcal{J} \varphi_{d+1}^{[i]}. \quad (2.34)$$

Simultaneously Hypothesis 2.1 guarantees the existence of a unique solution $z^{[1]} \in \mathbb{C}(\tilde{\mathcal{I}}_z^+)^{2n}$ of the nonhomogeneous initial value problem

$$\mathcal{L}(z^{[1]})_k = \Psi_k h_k^{[1]}, \quad z_c^{[1]} = 0, \quad k \in \tilde{\mathcal{I}}_z.$$

Then, for all $i \in \{1, \dots, 2n\}$, the fact $\mathcal{L}(\varphi^{[i]})_k \equiv 0$ and identity (2.10) yield

$$\sum_{k=c}^d h_k^{[1]*} \Psi_k \varphi_k^{[i]} = \sum_{k=c}^d \{ \mathcal{L}^*(z^{[1]})_k \varphi_k^{[i]} - z_k^{[1]*} \mathcal{L}(\varphi^{[i]})_k \} = (z^{[1]}, \varphi^{[i]})_k \Big|_c^{d+1} = (z^{[1]}, \varphi^{[i]})_{d+1}. \quad (2.35)$$

Upon combining (2.34) and (2.35) we obtain $z_{d+1}^{[1]} = \beta$, which means that $z^{[1]}$ solves the boundary value problem

$$\mathcal{L}(z^{[1]})_k = \Psi_k h_k^{[1]}, \quad z_c^{[1]} = 0, \quad z_{d+1}^{[1]} = \beta, \quad k \in \tilde{\mathcal{I}}_z.$$

Similarly, the nonhomogeneous system of algebraic equations $\omega^* A = \alpha^* \mathcal{J} \Phi_c$ has a unique solution $\omega = (\omega_1, \dots, \omega_{2n})^\top \in \mathbb{C}^{2n}$. Then with $h_k^{[2]} := \Phi_k \omega$, $k \in \tilde{\mathcal{I}}_z$, we can calculate that $z^{[2]} \in \mathbb{C}(\tilde{\mathcal{I}}_z^+)^{2n}$, being the unique solution of

$$\mathcal{L}(z^{[2]})_k = -\Psi_k h_k^{[2]}, \quad z_{d+1}^{[2]} = 0, \quad k \in \tilde{\mathcal{I}}_z,$$

also satisfies $z_c^{[2]} = \alpha$; i.e., it solves the boundary value problem

$$\mathcal{L}(z^{[2]})_k = -\Psi_k h_k^{[2]}, \quad z_c^{[2]} = \alpha, \quad z_{d+1}^{[2]} = 0, \quad k \in \tilde{\mathcal{I}}_z.$$

Thus, $z_k := z_k^{[1]} + z_k^{[2]}$, $k \in \tilde{\mathcal{I}}_z^+$, i.e., $z \in \mathbb{C}(\tilde{\mathcal{I}}_z^+)^{2n}$, solves the boundary value problem (2.32) with $f_k := h_k^{[1]} - h_k^{[2]}$ for $k \in \tilde{\mathcal{I}}_z$, i.e., $f \in \mathbb{C}(\tilde{\mathcal{I}}_z)^{2n}$. ■

2.2. Linear relations. The theory of linear relations has been established as a suitable tool for the study of multi-valued or non-densely defined linear operators in a Hilbert space. Its history goes back to [1] and the results were further developed e.g. in [11, 14, 15, 21]. In this subsection we recall the most relevant results from the theory of linear relations. A (closed) linear relation \mathcal{T} in a Hilbert space \mathcal{H} over \mathbb{C} with the inner product $\langle \cdot, \cdot \rangle$ is a (closed) linear subspace of the product space $\mathcal{H}^2 := \mathcal{H} \times \mathcal{H}$, i.e., the Hilbert space of all ordered pairs $\{z, f\}$ such that $z, f \in \mathcal{H}$. By $\text{dom } \mathcal{T}$, $\ker \mathcal{T}$, and $\overline{\mathcal{T}}$ we mean, respectively, the domain of \mathcal{T} , i.e., $\text{dom } \mathcal{T} := \{z \in \mathcal{H} \mid \{z, f\} \in \mathcal{T}\}$, the kernel of \mathcal{T} , i.e., $\ker \mathcal{T} := \{z \in \mathcal{H} \mid \{z, 0\} \in \mathcal{T}\}$, and the closure of \mathcal{T} . The sum $\mathcal{T} + \mathcal{U}$ and the algebraic sum $\mathcal{T} \dot{+} \mathcal{U}$ are defined as

$$\begin{aligned} \mathcal{T} + \mathcal{U} &:= \{\{z, f + g\} \mid \{z, f\} \in \mathcal{T}, \{z, g\} \in \mathcal{U}\}, \\ \mathcal{T} \dot{+} \mathcal{U} &:= \{\{z + y, f + g\} \mid \{z, f\} \in \mathcal{T}, \{y, g\} \in \mathcal{U}\}. \end{aligned}$$

The adjoint \mathcal{T}^* of the linear relation \mathcal{T} is the closed linear relation defined by

$$\mathcal{T}^* := \{\{y, g\} \in \mathcal{H}^2 \mid \langle z, g \rangle = \langle f, y \rangle \text{ for all } \{z, f\} \in \mathcal{T}\}.$$

A linear relation \mathcal{T} is said to be symmetric (or Hermitian) if $\mathcal{T} \subseteq \mathcal{T}^*$, and it is said to be self-adjoint if $\mathcal{T}^* = \mathcal{T}$. A symmetric linear relation \mathcal{T}_1 is said to be a self-adjoint extension of \mathcal{T} if $\mathcal{T} \subseteq \mathcal{T}_1$ and $\mathcal{T}_1^* = \mathcal{T}_1$. For $\lambda \in \mathbb{C}$ we define

$$\begin{aligned} \mathcal{T} - \lambda I &:= \{\{z, f - \lambda z\} \in \mathcal{H}^2 \mid \{z, f\} \in \mathcal{T}\}, \\ M_\lambda(\mathcal{T}) &:= \ker(\mathcal{T}^* - \lambda I) = \{z \in \mathcal{H} \mid \{z, \lambda z\} \in \mathcal{T}^*\}. \end{aligned}$$

The number $d_\lambda(\mathcal{T}) := \dim M_\lambda(\mathcal{T})$ is called the deficiency index of \mathcal{T} at λ and the subspace

$$\mathcal{M}_\lambda(\mathcal{T}) := \{\{z, \lambda z\} \in \mathcal{T}^*\}$$

denotes the defect space. It is known that the value of $d_\lambda(\mathcal{T})$ is constant in the upper and lower half plane of \mathbb{C} , i.e., for $\lambda \in \mathbb{C}_+$ and $\lambda \in \mathbb{C}_-$. Hence we define the positive and negative deficiency indices as $d_\pm(\mathcal{T}) := d_{\pm i}(\mathcal{T})$. If \mathcal{T} is a closed symmetric linear relation, then for every $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the following direct sum decomposition (a generalization of the von Neumann formula)

$$\mathcal{T}^* = \mathcal{T} \dot{+} \mathcal{M}_\lambda(\mathcal{T}) \dot{+} \mathcal{M}_{\bar{\lambda}}(\mathcal{T}) \quad (2.36)$$

holds, where the sum $\dot{+}$ is orthogonal for $\lambda = \pm i$; e.g. [26, Proposition 2.22]. Moreover, for a closed symmetric linear relation \mathcal{T} there is a self-adjoint extension if and only if $d_+(\mathcal{T}) = d_-(\mathcal{T})$, see [11, Corollary, pg. 34].

The main results concerning the characterization of all self-adjoint extensions of the minimal linear relation associated with system (S_λ) are obtained by applying the Glazman–Krein–Naimark theory for linear relations, which was established in [32].

A complex linear space \mathcal{S} with a complex-valued function $[\cdot] : \mathcal{S} \times \mathcal{S} \rightarrow \mathbb{C}$ is called pre-symplectic if it possesses the conjugate bilinear and skew-Hermitian properties, i.e., for all $P, Q, R \in \mathcal{S}$ and $\alpha \in \mathbb{C}$ we have

$$\begin{aligned} [P : Q + R] &= [P : Q] + [P : R], & [P + Q : R] &= [P : R] + [Q : R], \\ [\alpha P : Q] &= \alpha [P : Q], & [P : \alpha Q] &= \bar{\alpha} [P : Q], \\ [P : Q] &= -\overline{[Q : P]}; \end{aligned}$$

see [18] for more details. If we put $\mathcal{S} = \mathcal{H}^2$ and

$$[\{z, f\} : \{u, g\}] := \langle f, u \rangle - \langle z, g \rangle$$

for $\{z, f\}, \{u, g\} \in \mathcal{H}^2$, then \mathcal{S} and $[\cdot]$ form the pre-symplectic space.

For a symmetric linear relation $\mathcal{T} \subseteq \mathcal{H}^2$ we have

$$[\mathcal{T} : \mathcal{T}] = 0 = [\mathcal{T} : \mathcal{T}^*], \quad \overline{\mathcal{T}} = \{\{z, f\} \in \mathcal{T}^* \mid [\{z, f\} : \mathcal{T}^*] = 0\}; \quad (2.37)$$

see [32, Theorem 3.5]. If, in addition, the linear relation \mathcal{T} is closed and $d := d_+(\mathcal{T}) = d_-(\mathcal{T})$, then the set $\{\beta_j\}_{j=1}^d$ with $\beta_j \in \mathcal{T}^*$ for $j \in \{1, \dots, d\}$ such that

- (i) β_1, \dots, β_d are linearly independent in \mathcal{T}^* modulo \mathcal{T} ,
- (ii) $[\beta_j : \beta_i] = 0$ for all $i, j \in \{1, \dots, d\}$,

is called GKN-set for the pair of linear relations $(\mathcal{T}, \mathcal{T}^*)$. The following theorem provides the necessary and sufficient conditions for a linear relation $\mathcal{T}_1 \subseteq \mathcal{H}^2$ being a self-adjoint extension of \mathcal{T} (see [32, Theorem 4.7]).

Theorem 2.11. *Let $\mathcal{T} \subseteq \mathcal{H}^2$ be a closed symmetric linear relation such that $d_+(\mathcal{T}) = d_-(\mathcal{T}) = d$. A subspace $\mathcal{T}_1 \subseteq \mathcal{H}^2$ is a self-adjoint extension of \mathcal{T} if and only if there exists GKN-set $\{\beta_j\}_{j=1}^d$ for $(\mathcal{T}, \mathcal{T}^*)$ such that*

$$\mathcal{T}_1 = \{F \in \mathcal{T}^* \mid [F : \beta_j] = 0 \text{ for all } j = 1, \dots, d\}. \quad (2.38)$$

A linear relation \mathcal{T} is called semibounded below, if there exists $a \in \mathbb{R}$ such that

$$\langle z, f \rangle \geq a \langle z, z \rangle \text{ for all } \{z, f\} \in \mathcal{T}. \quad (2.39)$$

The number $m(\mathcal{T}) := \sup\{a \in \mathbb{R} \mid (2.39) \text{ holds}\}$ is called the lower bound of \mathcal{T} . If $m(\mathcal{T}) > 0$, the linear relation \mathcal{T} is said to be positive. Then, by analogy with the case of densely defined positive symmetric operators (see [12, Theorem 5]), the smallest and largest self-adjoint extensions of a positive symmetric linear relation are respectively known as the Krein–von Neumann (or soft) extension \mathcal{T}_K and the Friedrichs (or hard) extension \mathcal{T}_F . In particular, if \mathcal{T} is closed and $m(\mathcal{T}) > 0$, then the Krein–von Neumann extension admits the representation

$$\mathcal{T}_K = \mathcal{T} \dot{+} (\ker \mathcal{T}^* \times \{0\}) \quad (2.40)$$

(see [12, Corollary 1] and also [22]).

3. MAIN RESULTS

Since the weight matrix Ψ is assumed to be only positive semidefinite in Hypothesis 2.1, the space ℓ_Ψ^2 is not a Hilbert space. Hence we need to consider the Hilbert space of equivalence classes. It is the quotient space obtained by factoring out the kernel of the semi-norm $\|\cdot\|_\Psi$, i.e., the space

$$\tilde{\ell}_\Psi^2 = \tilde{\ell}_\Psi^2(\mathcal{I}_\mathbb{Z}) := \ell_\Psi^2 / \{z \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n} \mid \|z\|_\Psi = 0\}$$

with the inner product $\langle \tilde{z}, \tilde{f} \rangle_\Psi := \langle z, f \rangle_\Psi$, where z and f are elements of the equivalence classes $\tilde{z}, \tilde{f} \in \tilde{\ell}_\Psi^2$. Note that the value $\|\tilde{z}\|_\Psi$ for $z \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n}$ does not depend on z_{N+1} in the case of $\mathcal{I}_\mathbb{Z}$ being a finite discrete interval, which implies that the sequences $z, y \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n}$ such that $z_k \neq y_k$ only for $k = N + 1$, belong to the same equivalence class. We also introduce the space $\ell_{\Psi,0}^2$ as

$$\ell_{\Psi,0}^2 := \begin{cases} \{z \in \mathbb{C}_0(\mathcal{I}_\mathbb{Z}^+)^{2n} \mid z_0 = 0\} & \text{if } N = \infty, \\ \{z \in \mathbb{C}_0(\mathcal{I}_\mathbb{Z}^+)^{2n} \mid z_0 = 0, z_{N+1} = 0\} & \text{if } N \in \mathbb{N} \cup \{0\}. \end{cases}$$

Moreover, the corresponding function $[\cdot] : \tilde{\ell}_\Psi^{2 \times 2} \times \tilde{\ell}_\Psi^{2 \times 2} \rightarrow \mathbb{C}$ for the pre-symplectic space associated with $\tilde{\ell}_\Psi^{2 \times 2} := \tilde{\ell}_\Psi^2 \times \tilde{\ell}_\Psi^2$ is given by

$$[\{\tilde{z}, \tilde{f}\} : \{\tilde{w}, \tilde{g}\}] := \langle \tilde{f}, \tilde{w} \rangle_\Psi - \langle \tilde{z}, \tilde{g} \rangle_\Psi.$$

Linear relations associated with system (S_λ) were introduced and studied in [10, Section 5]. The maximal linear relation in $\tilde{\ell}_\Psi^{2 \times 2}$ is defined as

$$T_{\max} := \{\{\tilde{z}, \tilde{f}\} \in \tilde{\ell}_\Psi^{2 \times 2} \mid \text{there exists } u \in \tilde{z} \text{ such that } \mathcal{L}(u)_k = \Psi_k f_k \text{ for all } k \in \mathcal{I}_\mathbb{Z}\}.$$

Observe that the above definition does not depend on the particular choice of $f \in \tilde{f}$. Moreover, Hypothesis 2.4 is satisfied if and only if for any $\{\tilde{z}, \tilde{f}\} \in T_{\max}$ there exists unique $u \in \tilde{z}$ such that $\mathcal{L}(u)_k = \Psi_k f_k$ for all $k \in \mathcal{I}_\mathbb{Z}$, see [10, Theorem 5.2]. Henceforth, this unique element shall be denoted as \hat{z} . Then identity (2.11) yields for any $\{\tilde{z}, \tilde{f}\}, \{\tilde{w}, \tilde{g}\} \in T_{\max}$ that

$$[\{\tilde{z}, \tilde{f}\} : \{\tilde{w}, \tilde{g}\}] = \langle f, \hat{w} \rangle_\Psi - \langle \hat{z}, g \rangle_\Psi = (\hat{z}, \hat{w})_k \Big|_0^{N+1}, \quad (3.1)$$

where $f \in \tilde{f}$ and $g \in \tilde{g}$ are arbitrary representatives. Thus, under Hypothesis 2.4, we obtain from Lemma 2.10 the following statement, compare with [31, Remark 3.2] and [33, Lemma 3.3].

Lemma 3.1. *Let Hypothesis 2.4 be satisfied. Then for any pairs $\{\tilde{z}, \tilde{f}\}, \{\tilde{w}, \tilde{g}\} \in T_{\max}$ there exists $\{\tilde{y}, \tilde{h}\} \in T_{\max}$ such that*

$$\hat{y}_k = \begin{cases} \hat{z}_k, & k \in [0, c]_\mathbb{Z} \cap \mathcal{I}_\mathbb{Z}, \\ \hat{w}_k, & k \in [d+1, \infty)_\mathbb{Z} \cap \mathcal{I}_\mathbb{Z}^+, \end{cases}$$

where $c \in [0, a]_\mathbb{Z} \cap \mathcal{I}_\mathbb{Z}$, $d \in [b, \infty)_\mathbb{Z} \cap \mathcal{I}_\mathbb{Z}^+$ with a, b determining the interval $\mathcal{I}_\mathbb{Z}^\mathbb{D}$ in Hypothesis 2.4.

In particular, for $i \in \{1, \dots, 2n\}$ there exists $\{\tilde{z}^{[i]}, \tilde{f}^{[i]}\} \in T_{\max}$ such that $\hat{z}_0^{[i]} = e_i$ and $\hat{z}_k^{[i]} = 0$ for $k \in [d+1, \infty)_\mathbb{Z} \cap \mathcal{I}_\mathbb{Z}^+$, where $e_i = (0, \dots, 1, \dots, 0)^\top \in \mathbb{C}^{2n}$ is the i -th canonical unit vector. If, in addition, $N \in \mathbb{N} \cup \{0\}$, i.e., $\mathcal{I}_\mathbb{Z}$ is a finite discrete interval, then there exists $\{\tilde{y}^{[i]}, \tilde{h}\} \in T_{\max}$ such that $\hat{y}_{N+1}^{[i]} = e_i$ and $\hat{y}_k^{[i]} = 0$ for $k \in [0, c]_\mathbb{Z} \cap \mathcal{I}_\mathbb{Z}$.

Proof. Let $\tilde{\mathcal{I}}_\mathbb{Z}$ be a finite discrete interval as in Lemma 2.10, the pairs $\{\tilde{z}, \tilde{f}\}, \{\tilde{w}, \tilde{g}\} \in T_{\max}$ be arbitrary, and define $\alpha := \hat{z}_c$, $\beta := \hat{w}_{d+1}$. Then, by the latter lemma there exist sequences $l \in \mathbb{C}(\tilde{\mathcal{I}}_\mathbb{Z}^+)^{2n}$ and $v \in \mathbb{C}(\tilde{\mathcal{I}}_\mathbb{Z}^+)^{2n}$ such that

$$\mathcal{L}(v)_k = \Psi_k l_k, \quad v_c = \alpha, \quad v_{d+1} = \beta, \quad k \in \tilde{\mathcal{I}}_\mathbb{Z}.$$

Putting

$$y_k := \begin{cases} \hat{z}_k, & k \in [0, c]_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}, \\ v_k, & k \in [c+1, d]_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}, \\ \hat{w}_k, & k \in [d+1, \infty)_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}^+ \end{cases} \quad h_k := \begin{cases} f_k, & k \in [0, c-1]_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}, \\ l_k, & k \in [c, d]_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}, \\ g_k, & k \in [d+1, \infty)_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}, \end{cases}$$

it can be verified by a direct calculation that $y, g \in \ell_{\Psi}^2$ and that they satisfy $\mathcal{L}(y)_k = \Psi_k h_k$ for $k \in \mathcal{I}_{\mathbb{Z}}$, i.e., $\{\tilde{y}, \tilde{h}\} \in T_{\max}$ with $\hat{y}_k \equiv y_k$. The second part of the statement follows directly from Lemma 2.10. \blacksquare

The minimal linear relation is defined as $T_{\min} := \overline{T_0}$, where T_0 is the pre-minimal linear relation

$$T_0 := \{ \{\tilde{z}, \tilde{f}\} \in \tilde{\ell}_{\Psi}^{2 \times 2} \mid \text{there exists } u \in \tilde{z} \cap \ell_{\Psi,0}^2 \text{ such that } \mathcal{L}(u)_k = \Psi_k f_k \text{ for all } k \in \mathcal{I}_{\mathbb{Z}} \}.$$

It was shown in [10, Theorem 5.10] that

$$T_0^* = T_{\min}^* = T_{\max}, \quad (3.2)$$

which implies that T_{\min} is a closed and symmetric linear relation. Moreover, the following theorem provides a more explicit characterization of T_{\min} ; cf. [31, Theorem 3.2].

Theorem 3.2. *Let Hypothesis 2.4 be satisfied. Then,*

$$T_{\min} = \{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid \hat{z}_0 = 0 = (\hat{z}, \hat{w})_{N+1} \text{ for all } \tilde{w} \in \text{dom } T_{\max} \}, \quad (3.3)$$

which in the case of $\mathcal{I}_{\mathbb{Z}}$ being a finite discrete interval reduces to

$$T_{\min} = \{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid \hat{z}_0 = 0 = \hat{z}_{N+1} \}. \quad (3.4)$$

Proof. Since $T_{\min} = \overline{(T_{\min})}$ by the definition, identities (2.37), (3.1), and (3.2) yield

$$T_{\min} = \{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid (\hat{z}, \hat{w})_k \big|_0^{N+1} = 0 \text{ for all } \hat{w} \in \text{dom } T_{\max} \}. \quad (3.5)$$

Let T be the linear relation on the right-hand side of (3.3). Then, it is obvious that $T \subseteq T_{\min}$. On the other hand, let $\{\tilde{z}, \tilde{f}\} \in T_{\min}$ be fixed. Then, $(\hat{z}, \hat{w})_k \big|_0^{N+1} = 0$ for all $\hat{w} \in \text{dom } T_{\max}$ by (3.5). By Lemma 3.1, for any $\{\tilde{w}, \tilde{g}\} \in T_{\max}$ there exists $\{\tilde{y}, \tilde{h}\} \in T_{\max}$ such that $\hat{y}_k = 0$ for $k \in [0, c]_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}$ and $\hat{y}_k = \hat{w}_k$ for $k \in [d+1, \infty)_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}^+$. Hence $(\hat{z}, \hat{w})_0 = (\hat{z}, \hat{w})_{N+1} = 0$ for all $\hat{w} \in \text{dom } T_{\max}$. From the second part of Lemma 3.1 we get $\hat{z}_0 = 0$, because there exists $\{\tilde{z}^{[i]}, \tilde{f}^{[i]}\} \in T_{\max}$ such that $\hat{z}_0^{[i]} = e_i$. Therefore, $T = T_{\min}$. If, in addition, $\mathcal{I}_{\mathbb{Z}}$ is a finite discrete interval, i.e., $N \in \mathbb{N}$, then $\text{dom } T_{\max}$ contains also \tilde{y} such that $\hat{y}_{N+1} = e^{[i]}$, $i \in \{1, \dots, 2n\}$, by the last part of Lemma 3.1. Hence equality (3.4) holds. \blacksquare

By [10, Corollary 5.12], Hypothesis 2.4 is equivalent with the equality $q(\lambda) = d_{\lambda}(T_{\min})$, which means that the number of the linearly independent square summable solutions of (S_{λ}) is constant in \mathbb{C}_+ and \mathbb{C}_- . Therefore the numbers $q_+ := q(\lambda)$ for $\lambda \in \mathbb{C}_+$ and $q_- := q(\lambda)$ for $\lambda \in \mathbb{C}_-$ are well-defined for $q(\lambda)$ given in (2.18). Let $\lambda_0 \in \mathbb{C}_+$ be fixed. Then system (S_{λ_0}) has q_+ linearly independent square summable solutions, which we denote as $v^{[1]}(\lambda_0), \dots, v^{[q_+]}(\lambda_0)$, and similarly system $(S_{\bar{\lambda}_0})$ has q_- linearly independent square summable solutions, which we denote as $w^{[1]}(\bar{\lambda}_0), \dots, w^{[q_-]}(\bar{\lambda}_0)$. Let

$$\varphi_k^{[i]} := v_k^{[i]}(\lambda_0), \quad \varphi_k^{[j+q_+]} := w_k^{[j]}(\bar{\lambda}_0), \quad i = 1, \dots, q_+, \quad j = 1, \dots, q_-, \quad k \in \mathcal{I}_{\mathbb{Z}}^+, \quad (3.6)$$

and $\Phi_k := (\Phi_k^+, \Phi_k^-) \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n \times p}$, where $\Phi_k^+ := (\varphi_k^{[1]}, \dots, \varphi_k^{[q_+]})$ and $\Phi_k^- := (\varphi_k^{[1+q_+]}, \dots, \varphi_k^{[p]})$ with $2n \leq p := q_+ + q_- \leq 4n$. Then for $i \in \{1, \dots, q_+\}$ and $j \in \{q_+ + 1, \dots, p\}$ we have $\{\tilde{\varphi}^{[i]}, \lambda_0 \tilde{\varphi}^{[i]}\} \in T_{\max}$ and $\{\tilde{\varphi}^{[j]}, \lambda_0 \tilde{\varphi}^{[j]}\} \in T_{\max}$ with $\hat{\varphi}^{[l]} \equiv \varphi^{[l]}$ for $l = 1, \dots, p$. We also define the matrix

$$\Omega = \begin{pmatrix} \Omega^{[1,1]} & \Omega^{[1,2]} \\ \Omega^{[2,1]} & \Omega^{[2,2]} \end{pmatrix} := \begin{pmatrix} (\varphi^{[1]}, \varphi^{[1]})_{N+1} & \dots & (\varphi^{[1]}, \varphi^{[p]})_{N+1} \\ \vdots & \ddots & \vdots \\ (\varphi^{[p]}, \varphi^{[1]})_{N+1} & \dots & (\varphi^{[p]}, \varphi^{[p]})_{N+1} \end{pmatrix} \in \mathbb{C}^{p \times p}, \quad (3.7)$$

where $\Omega^{[1,2]} \in \mathbb{C}^{q_+ \times q_-}$. Note that the elements $\omega_{ij} := (\varphi^{[i]}, \varphi^{[j]})_{N+1}$ exist finite for all $i, j = 1, \dots, p$ by identity (2.11). Moreover, from (2.7) one easily concludes that the matrix $\Omega^{[1,2]}$ consists of the elements $(\varphi^{[i]}, \varphi^{[j]})_{N+1} = (\varphi^{[i]}, \varphi^{[j]})_0$ for $i \in \{1, \dots, q_+\}$ and $j \in \{q_+ + 1, \dots, p\}$.

Upon combining (3.2) and (2.36) we get that any $\{\tilde{z}, \tilde{f}\} \in T_{\max}$ can be written as

$$\hat{z}_k = \hat{y}_k + \sum_{j=1}^p \xi_j \varphi_k^{[j]}, \quad k \in \mathcal{I}_\mathbb{Z}^+, \quad (3.8)$$

where $\hat{y} \in \text{dom } T_{\min}$ and $\xi_1, \dots, \xi_p \in \mathbb{C}$ are determined uniquely. Especially, for $\{\tilde{z}^{[i]}, \tilde{f}^{[i]}\} \in T_{\max}$ (see Lemma 3.1), we get the unique expression

$$\hat{z}_k^{[i]} = \hat{y}_k^{[i]} + \sum_{j=1}^p \xi_{i,j} \varphi_k^{[j]}, \quad k \in \mathcal{I}_\mathbb{Z}^+, \quad i = 1, \dots, 2n. \quad (3.9)$$

If we put $Z_k := (\hat{z}_k^{[1]}, \dots, \hat{z}_k^{[2n]})$ for $k \in \mathcal{I}_\mathbb{Z}^+$, then identity (3.9) implies

$$Z_k = Y_k + \Phi_k \Xi^\top, \quad (3.10)$$

where $Y_k := (\hat{y}_k^{[1]}, \dots, \hat{y}_k^{[2n]}) \in \mathbb{C}(\mathcal{I}_\mathbb{Z}^+)^{2n \times 2n}$ and the matrix $\Xi \in \mathbb{C}^{2n \times p}$ consists of the elements $\xi_{i,j}$. In particular, for $k = 0$ we obtain $I = Y_0 + \Phi_0 \Xi^\top$, which together with (3.3) yields $I = \Phi_0 \Xi^\top$, i.e., $\text{rank } \Xi = 2n$ by the second inequality in (2.2). From the definition of $\hat{z}^{[i]}$, its expression in (3.9), and identity (3.3) we have

$$0 = (\hat{z}^{[i]}, \varphi^{[l]})_{N+1} = (\hat{y}^{[i]}, \varphi^{[l]})_{N+1} + \sum_{j=1}^p \overline{\xi_{i,j}} (\varphi^{[j]}, \varphi^{[l]})_{N+1} = \sum_{j=1}^p \overline{\xi_{i,j}} (\varphi^{[j]}, \varphi^{[l]})_{N+1}$$

for all $i \in \{1, \dots, 2n\}$ and any $l \in \{1, \dots, p\}$, i.e., $\overline{\Xi} \Omega = 0$. Since $\text{rank } \Xi = 2n$, the first inequality in (2.2) implies

$$\text{rank } \Omega \leq p - 2n.$$

On the other hand, the equality $\Omega^{[1,2]} = \Phi_0^{+*} \mathcal{J} \Phi_0^-$ and the first inequality in (2.2) yield

$$\text{rank } \Omega^{[1,2]} \geq p - 2n.$$

Therefore, $\text{rank } \Omega = p - 2n = \text{rank } \Omega^{[1,2]}$. Since $p - 2n \leq q_+$ and $p - 2n \leq q_-$, we may assume, without loss of generality, that $\varphi^{[1]}, \dots, \varphi^{[q_+]}$ are arranged such that

$$\text{rank } \Omega_{p-2n, q_-}^{[1,2]} = p - 2n. \quad (3.11)$$

The main result concerning the characterization of all self-adjoint extension of T_{\min} is stated in the following theorem and its proof is given in Section 4; cf. [31, Theorem 5.7]. Recall that for the existence of a self-adjoint extension it is essential to assume $q_+ = q_-$.

Theorem 3.3. *Let Hypothesis 2.4 be satisfied, equality $q_+ = q_- =: q$ hold and assume that the solutions $\varphi^{[1]}, \dots, \varphi^{[q]}$ are arranged such that (3.11) holds. Then a linear relation $T \subseteq \tilde{\ell}_{\Psi}^{2 \times 2}$ is a self-adjoint extension of T_{\min} if and only if there exist matrices $M \in \mathbb{C}^{q \times 2n}$ and $L \in \mathbb{C}^{q \times (2q-2n)}$ such that*

$$\text{rank}(M, L) = q, \quad M \mathcal{J} M^* - L \Omega_{2q-2n} L^* = 0, \quad (3.12)$$

and

$$T = \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid M \hat{z}_0 - L \begin{pmatrix} (\varphi^{[1]}, \hat{z})_{N+1} \\ \vdots \\ (\varphi^{[2q-2n]}, \hat{z})_{N+1} \end{pmatrix} = 0 \right\}. \quad (3.13)$$

Remark 3.4. If, in addition to the assumptions of Theorem 3.3, there exists $\nu \in \mathbb{R}$ such that (S_{ν}) has q linearly independent square summable solutions (suppressing the argument ν) $\Theta^{[1]}, \dots, \Theta^{[q]}$, then the statement of Theorem 3.3 can be formulated by using these solutions, which are (without loss of generality) arranged such that the submatrix Υ_{2q-2n} has the full rank, where

$$\Upsilon := \begin{pmatrix} (\Theta^{[1]}, \Theta^{[1]})_{N+1} & \dots & (\Theta^{[1]}, \Theta^{[q]})_{N+1} \\ \vdots & \ddots & \vdots \\ (\Theta^{[q]}, \Theta^{[1]})_{N+1} & \dots & (\Theta^{[q]}, \Theta^{[q]})_{N+1} \end{pmatrix},$$

see Lemma 4.3. Moreover, the Wronskian-type identity (2.7) yields that $\Upsilon = \Theta_0^* \mathcal{J} \Theta_0$, where $\Theta_k := (\Theta_k^{[1]}, \dots, \Theta_k^{[q]})$ for $k \in \mathcal{I}_{\mathbb{Z}}^+$.

In the next part we discuss several special cases of Theorem 3.3. If system (S_{λ}) is in the limit point case for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$, i.e., $q_+ = q_- = n$, then the boundary conditions at $N+1$ (which is necessary equal to ∞) are superfluous as stated in the following corollary; cf. [31, Theorem 5.9]. *This situation occurs, e.g., when the assumptions of Theorem 2.7 are satisfied.* The proof follows directly from Theorem 3.3.

Corollary 3.5. *Let Hypothesis 2.4 be satisfied and $q_+ = q_- = n$ hold. Then a linear relation $T \subseteq \tilde{\ell}_{\Psi}^{2 \times 2}$ is a self-adjoint extension of T_{\min} if and only if there exists a matrix $M \in \mathbb{C}^{n \times 2n}$ such that*

$$\text{rank } M = n, \quad M \mathcal{J} M^* = 0,$$

and

$$T = \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid M \hat{z}_0 = 0 \right\}.$$

If there exists $\lambda_0 \in \mathbb{C}$ with the property $q(\lambda_0) = 2n$, then system (S_{λ}) is in the limit circle case for all $\lambda \in \mathbb{C}$, i.e., $q_+ = q_- = 2n$, see Remark 2.6. Hence for any $\nu \in \mathbb{R}$ there exist solutions (suppressing the argument ν) $\Theta^{[1]}, \dots, \Theta^{[2n]}$ of system (S_{ν}) , which are linearly independent, square summable, and the fundamental matrix Θ_k satisfies $\Theta_0 = I$, which implies $\Upsilon = \mathcal{J}$, i.e., $\text{rank } \Upsilon = 2n$, see Remark 3.4. Upon combining the latter remark and Theorem 3.3 we obtain the following result; cf. [31, Theorem 5.10].

Corollary 3.6. *Let Hypothesis 2.4 be satisfied, assume that there exists a number $\lambda_0 \in \mathbb{C}$ such that $q(\lambda_0) = 2n$, and $\nu \in \mathbb{R}$ be fixed. Let Θ_k be the fundamental matrix of system (S_{ν}) satisfying $\Theta_0 = I$ and denote its columns by $\Theta^{[1]}, \dots, \Theta^{[2n]}$, i.e., $\Theta_k = (\Theta_k^{[1]}, \dots, \Theta_k^{[2n]})$. Then a linear relation $T \subseteq \tilde{\ell}_{\Psi}^{2 \times 2}$ is a self-adjoint extension of T_{\min} if and only if there exist matrices $M, L \in \mathbb{C}^{2n \times 2n}$ such that*

$$\text{rank}(M, L) = 2n, \quad M \mathcal{J} M^* - L \mathcal{J} L^* = 0, \quad (3.14)$$

and

$$T = \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid M\hat{z}_0 - L \begin{pmatrix} (\Theta^{[1]}, \hat{z})_{N+1} \\ \vdots \\ (\Theta^{[2n]}, \hat{z})_{N+1} \end{pmatrix} = 0 \right\}. \quad (3.15)$$

Especially, if $\mathcal{I}_{\mathbb{Z}}$ is a finite discrete interval, then the equality $q(\lambda) = 2n$ is trivially satisfied for any $\lambda \in \mathbb{C}$. Therefore we get from Corollary 3.6 yet one more special case of Theorem 3.3.

Corollary 3.7. *Let $\mathcal{I}_{\mathbb{Z}}$ be a finite discrete interval and Hypothesis 2.4 be satisfied. Then a linear relation $T \subseteq \tilde{\ell}_{\Psi}^{2 \times 2}$ is a self-adjoint extension of T_{\min} if and only if there exist matrices $M, L \in \mathbb{C}^{2n \times 2n}$ such that*

$$\text{rank}(M, L) = 2n, \quad M\mathcal{J}M^* - L\mathcal{J}L^* = 0, \quad (3.16)$$

and

$$T = T_{M,L} := \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid M\hat{z}_0 - L\hat{z}_{N+1} = 0 \right\}. \quad (3.17)$$

Proof. By Corollary 3.6 every self-adjoint extension of T_{\min} can be expressed as in (3.15) with matrices $M, L \in \mathbb{C}^{2n \times 2n}$ satisfying (3.14). If we put $\tilde{L} := L\Phi_{N+1}^*\mathcal{J} \in \mathbb{C}^{2n \times 2n}$, then M, \tilde{L} satisfies (3.16) and the linear relation in (3.15) can be written as $T_{M, \tilde{L}}$. ■

One can easily observe that a linear relation $T_{M,L}$, i.e., the linear relation given by (3.17) with $M, L \in \mathbb{C}^{2n \times 2n}$ satisfying (3.16), is the same as a linear relation $T_{\mathcal{M}, \mathcal{L}}$, where $\mathcal{M} := CM$ and $\mathcal{L} := CL$ for an arbitrary invertible matrix $C \in \mathbb{C}^{2n \times 2n}$. We show that the converse is also true (see Remark 3.12(i)). Moreover, it is well known that all self-adjoint extensions of operators associated with the regular second order Sturm–Liouville differential equations can be expressed by using the separated or coupled boundary conditions; e.g. [8]. In the last part of this section we show similar results for scalar symplectic systems on a finite interval, i.e., $n = 1$ and $N \in \mathbb{N}$, and provide a unique representation of all self-adjoint extensions of T_{\min} . The main assumptions for this treatment are summarized in the following hypothesis.

Hypothesis 3.8. The discrete interval $\mathcal{I}_{\mathbb{Z}}$ is finite, i.e., there exists $N \in \mathbb{N}$ such that $\mathcal{I}_{\mathbb{Z}} = [0, N]_{\mathbb{Z}}$, we have $n = 1$, Hypothesis 2.4 is satisfied, and the matrices $M, L \in \mathbb{C}^{2 \times 2}$ are such that (3.16) holds.

In this case, identity (3.16) implies either that $\text{rank } M = \text{rank } L = 2$, or that $\text{rank } M = \text{rank } L = 1$, which together yield the following dichotomy on the boundary conditions in (3.17).

Theorem 3.9. *Let Hypothesis 3.8 be satisfied. Then, the following hold.*

- (i) *A linear relation $T_{M,L}$ given through $M, L \in \mathbb{C}^{2 \times 2}$ with $\text{rank } M = 1 = \text{rank } L$ is a self-adjoint extension of T_{\min} if and only if $T_{M,L} = T_{P,Q} := \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid P\hat{z}_0 = 0 = Q\hat{z}_{N+1} \right\}$, where*

$$P = \begin{pmatrix} \cos \alpha_0 & \sin \alpha_0 \\ 0 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} 0 & 0 \\ -\sin \alpha_{N+1} & \cos \alpha_{N+1} \end{pmatrix}, \quad (3.18)$$

for a unique pair $\alpha_0, \alpha_{N+1} \in [0, \pi)$.

- (ii) *A linear relation $T_{M,L}$ given through $M, L \in \mathbb{C}^{2 \times 2}$ with $\text{rank } M = 2 = \text{rank } L$ is a self-adjoint extension of T_{\min} if and only if $T_{M,L} = T_{R,\beta} := \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid e^{i\beta} R\hat{z}_0 = \hat{z}_{N+1} \right\}$ with a unique $\beta \in [0, \pi)$ and a symplectic matrix $R \in \mathbb{R}^{2 \times 2}$.*

Proof. Since the pairs of matrices P, Q and $e^{i\beta} R, I$ satisfy (3.16), Corollary 3.7 implies that the linear relations $T_{P,Q}$ and $T_{R,\beta}$ are self-adjoint extensions of T_{\min} .

- (i) Let $T_{M,L}$ be a linear relation given through $M, L \in \mathbb{C}^{2 \times 2}$ satisfying (3.16) and with $\text{rank } M = 1 = \text{rank } L$. Since by (2.4) we have $\dim[\mathcal{R}(M) \cap \mathcal{R}(L)] = 0$, it follows that $M\xi = L\eta$ for some

$\xi, \eta \in \mathbb{C}^2$ if and only if $M\xi = 0 = L\eta$. Therefore, the boundary conditions in (3.17) can be expressed as $M\hat{z}_0 = 0 = L\hat{z}_{N+1}$. The rank condition implies that $M = ab^\top$ and $L = cd^\top$ for some vectors $a, b, c, d \in \mathbb{C}^2 \setminus \{0\}$. Then the equality $M\mathcal{J}M^* = 0 = L\mathcal{J}L^*$ does not depend on the vectors a, c and it is equivalent with $b^\top \mathcal{J} b = 0 = d^\top \mathcal{J} d$, which implies that b and d are (scalar) complex multiples of vectors from \mathbb{R}^2 . Therefore, without loss of generality, a, c may be chosen such that M, L can be written in the form as in (3.18) for some $\alpha_0, \alpha_{N+1} \in [0, \pi)$. The uniqueness follows from the fact that $\cotan \alpha = \cotan \beta$ with $\alpha, \beta \in (0, \pi)$ if and only if $\alpha = \beta$.

(ii) Finally, let $T_{M,L}$ be a linear relation given through $M, L \in \mathbb{C}^{2 \times 2}$ satisfying (3.16) and with $\text{rank } M = 2 = \text{rank } L$. Then the boundary conditions in (3.17) can be written as $\hat{z}_{N+1} = K\hat{z}_0$, where $K := L^{-1}M$. Upon applying the second equality in (3.16) we obtain that the matrix K is conjugate symplectic, i.e., $K\mathcal{J}K^* = \mathcal{J}$. Therefore, $K^{-1} = -\mathcal{J}K^*\mathcal{J}$ and $|\det K| = 1$, i.e., $\det K = e^{i\delta}$ for some $\delta \in [0, 2\pi)$, which implies $K^{-1} = e^{-i\delta} \text{adj}(K) = -e^{i\delta} \mathcal{J}K^\top \mathcal{J}$, i.e., $K^{*\top} = \overline{K} = e^{i\delta} K$. If we put $R := e^{-i\delta/2} K$, i.e., $K = e^{i\delta/2} R$, then $\overline{R} = R$ and $\det R = 1$, i.e., $R \in \mathbb{R}^{2 \times 2}$ is a symplectic matrix. Uniqueness can be verified by a direct calculation. \blacksquare

As an illustration of the last theorem we provide a description of the Krein–von Neumann extension of the minimal linear relation T_{\min} under Hypothesis 3.8.

Example 3.10. Assume that system (S_λ) is such that Hypothesis 3.8 holds and that the minimal linear relation T_{\min} is positive, i.e., there exists $c > 0$ such that $\langle \tilde{z}, \tilde{f} \rangle_\Psi \geq c \|\tilde{z}\|_\Psi$ for all $\{\tilde{z}, \tilde{f}\} \in T_{\min}$. Then the Krein–von Neumann self-adjoint extension of T_{\min} admits the representation given in (2.40), i.e.,

$$T_K = T_{\min} \dot{+} (\ker T_{\max} \times \{0\}).$$

We show that T_K can be also expressed as in the second part of Theorem 3.9 with a suitable matrix R and a number $\beta \in [0, 2\pi)$. By definition,

$$\ker T_{\max} = \{\tilde{z} \in \ell_\Psi^2 \mid \{\tilde{z}, \tilde{0}\} \in T_{\max}\},$$

i.e., \hat{z} solves (S_0) , i.e., $\mathcal{L}(\hat{z})_k = 0$ on $[0, N]_{\mathbb{Z}}$. Because all solutions of (S_0) are square summable in this case, Hypothesis 2.4 implies that $\dim \ker T_{\max} = 2$. If $\tilde{z} \in \text{dom } T_K$, then there exist $\tilde{y} \in \text{dom } T_{\min}$ and $\tilde{w} \in \ker T_{\max}$ such that $\tilde{z} = \tilde{y} + \tilde{w}$ or

$$\hat{z}_k = \hat{y}_k + \hat{w}_k \quad \text{for all } k \in [0, N+1]_{\mathbb{Z}}, \quad (3.19)$$

where $\hat{z} \in \tilde{z}$, $\hat{y} \in \tilde{y}$, and $\hat{w} \in \tilde{w}$ are the uniquely determined elements. Moreover, $\hat{y}_0 = 0 = \hat{y}_{N+1}$ by (3.4) and $\hat{w}_k = \alpha^{[1]} \hat{w}_k^{[1]} + \alpha^{[2]} \hat{w}_k^{[2]}$ for all $k \in [0, N+1]_{\mathbb{Z}}$, where $\hat{w}^{[1]}$ and $\hat{w}^{[2]}$ form a basis of $\ker T_{\max}$.

Let us define the matrix $\mathcal{G} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} := (\mathcal{S}_0 \times \mathcal{S}_1 \times \cdots \times \mathcal{S}_N)^{-1} \in \mathbb{C}^{2 \times 2}$. Then one easily concludes that the matrix \mathcal{G} is symplectic and every solution $z \in \mathbb{C}([0, N+1]_{\mathbb{Z}})^2$ of system (S_0) satisfies

$$z_{N+1} = \mathcal{G}z_0. \quad (3.20)$$

In the following construction we consider two cases: either $b \neq 0$ or $b = 0$.

First, assume that $b \neq 0$. Then there exist two solutions of system (S_0) such that

$$\hat{w}_0^{[1]} = \begin{pmatrix} 0 \\ 1/b \end{pmatrix}, \quad \hat{w}_0^{[2]} = \begin{pmatrix} 1 \\ -a/b \end{pmatrix}.$$

These solutions are obviously linearly independent and by (3.20) we have

$$\hat{w}_{N+1}^{[1]} = \begin{pmatrix} 1 \\ a/b \end{pmatrix}, \quad \hat{w}_{N+1}^{[2]} = \begin{pmatrix} 0 \\ c - da/b \end{pmatrix}.$$

If we take these two solutions as a basis of $\ker T_{\max}$, then (3.19) yields

$$\hat{z}_k = \hat{y}_k + \alpha^{[1]} \hat{w}_k^{[1]} + \alpha^{[2]} \hat{w}_k^{[2]} \quad \text{for all } k \in [0, N+1]_{\mathbb{Z}}.$$

Upon evaluating \hat{z}_k at $k = 0$ and $k = N+1$ we obtain

$$\hat{z}_0 = \begin{pmatrix} \alpha^{[2]} \\ \alpha^{[1]}/b - \alpha^{[2]}a/b \end{pmatrix}, \quad \hat{z}_{N+1} = \begin{pmatrix} \alpha^{[1]} \\ \alpha^{[1]}d/b + \alpha^{[2]}c - \alpha^{[2]}da/b \end{pmatrix},$$

which for $\hat{z}_k = \begin{pmatrix} \hat{x}_k \\ \hat{u}_k \end{pmatrix}$ implies $\alpha^{[1]} = \hat{x}_{N+1}$ and $\alpha^{[2]} = \hat{x}_0$. Therefore,

$$\begin{pmatrix} \hat{x}_{N+1} \\ \hat{x}_{N+1}d/b + \hat{x}_0c - \hat{x}_0da/b \end{pmatrix} = \hat{z}_{N+1} = \mathcal{G} \hat{z}_0 = \mathcal{G} \begin{pmatrix} \hat{x}_0 \\ \hat{x}_{N+1}/b - \hat{x}_0a/b \end{pmatrix}.$$

It means that $\hat{z} \in \text{dom } T_{R,\beta}$, where $\beta \in [0, \pi)$ is such that $e^{i\beta} = \sqrt{ad - bc}$, and $R = e^{-i\beta} \mathcal{G}$, i.e., $T_K \subseteq T_{R,\beta}$. On the other hand, T_K and $T_{R,\beta}$ are self-adjoint extensions of T_{\min} , thus $T_K = T_{R,\beta}$. Especially, if the coefficients a, b, c, d are real, then $T_{R,\beta} = T_{\mathcal{G},0}$.

If $b = 0$, then $\mathcal{G} = \begin{pmatrix} a & 0 \\ c & d \end{pmatrix}$ with $|ad| = 1$, i.e., $d \neq 0$. In this case we proceed in the same way with the basis of $\ker T_{\max}$ given by the solutions $\tilde{w}^{[1]}$ and $\tilde{w}^{[2]}$ of (S_0) such that

$$\hat{w}_0^{[1]} = \begin{pmatrix} 0 \\ 1/d \end{pmatrix}, \quad \hat{w}_0^{[2]} = \begin{pmatrix} 1 \\ -c/d \end{pmatrix}.$$

Then $\begin{pmatrix} \hat{x}_0 a \\ \hat{u}_{N+1} \end{pmatrix} = \hat{z}_{N+1} = \mathcal{G} \hat{z}_0 = \mathcal{G} \begin{pmatrix} \hat{x}_0 \\ \hat{u}_{N+1}/d - \hat{x}_0c/d \end{pmatrix}$. This shows (again) that $T_K = T_{R,\beta}$ with $\beta \in [0, \pi)$ being such that $e^{i\beta} = \sqrt{ad}$, and $R = e^{-i\beta} \mathcal{G}$.

In particular, let $\mathcal{S}_k = \begin{pmatrix} 1 & -b_k \\ 0 & 1 \end{pmatrix}$ and $\Psi_k = \begin{pmatrix} w_k & 0 \\ 0 & 0 \end{pmatrix}$ with $b_k > 0$ and $w_k > 0$ on $[0, N]_{\mathbb{Z}}$. This system satisfies Hypothesis 2.4 and corresponds to the second order Sturm–Liouville difference equation $-\Delta[p_k \Delta y_{k-1}(\lambda)] = \lambda w_k y_k(\lambda)$ with $b_k = 1/p_{k+1}$ (see Example 2.5(i)). Then $\mathcal{G} = \begin{pmatrix} 1 & \sum_{k=0}^N b_k \\ 0 & 1 \end{pmatrix}$ and by the previous part we have

$$T_K = \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid \hat{z} = \begin{pmatrix} \hat{x} \\ \hat{u} \end{pmatrix} \in \mathbb{C}([0, N+1]_{\mathbb{Z}})^2, \hat{u}_0 = \hat{u}_{N+1} = \left(\sum_{k=0}^N b_k \right)^{-1} \times (\hat{x}_{N+1} - \hat{x}_0) \right\}. \quad \blacktriangle$$

The boundary conditions in Theorem 3.9 include four particular cases. Namely, for $\alpha_0 = 0$ and $\alpha_{N+1} = \pi/2$ we get the Dirichlet boundary conditions $\hat{x}_0 = 0 = \hat{x}_{N+1}$, while for $\alpha_0 = \pi/2$ and $\alpha_{N+1} = 0$ we have the Neumann boundary conditions $\hat{u}_0 = 0 = \hat{u}_{N+1}$, where $\hat{z}_k = \begin{pmatrix} \hat{x}_k \\ \hat{u}_k \end{pmatrix}$. The choice $R = I$ and $\beta = 0$ yields the periodic boundary conditions $\hat{z}_0 = \hat{z}_{N+1}$ and the choice $R = I$ and $\beta = \pi$ leads to the antiperiodic boundary conditions $\hat{z}_0 = -\hat{z}_{N+1}$.

In the first part of the following theorem we show that any self-adjoint extension of T_{\min} can be described by using the matrices determining the Dirichlet and Neumann boundary conditions. For convenience, we introduce the general boundary trace map $\gamma_{M,L} : \mathbb{C}(\mathcal{I}_{\mathbb{Z}}^+)^2 \rightarrow \mathbb{C}^2$ as

$$\gamma_{M,L}(\hat{z}) := M\hat{z}_0 - L\hat{z}_{N+1},$$

see also [8]. Then $T_{M,L} = \{\{\tilde{z}, \tilde{f}\} \in T_{\max} \mid \gamma_{M,L}(\hat{z}) = 0\}$. Especially, for P, Q given in (3.18) we denote $\gamma_x := \gamma_{P,Q}$ for $\alpha_0 = 0, \alpha_{N+1} = \pi/2$, i.e., $\gamma_x(\hat{z}) = 0$ abbreviates the Dirichlet boundary conditions, and similarly $\gamma_u := \gamma_{P,Q}$ for $\alpha_0 = \pi/2, \alpha_{N+1} = 0$, i.e., $\gamma_u(\hat{z}) = 0$ abbreviates the Neumann boundary conditions. In the second part of this theorem we derive yet another equivalent representation of $T_{M,L}$, which possesses the uniqueness property.

Theorem 3.11. *Let Hypothesis 3.8 be satisfied. Then the following hold.*

- (i) A linear relation T is a self-adjoint extension of T_{\min} if and only if there exist matrices $F, G \in \mathbb{C}^{2 \times 2}$ such that

$$\text{rank}(F, G) = 2, \quad FG^* = GF^* \quad (3.21)$$

and

$$T = T_{F,G} := \{ \{ \tilde{z}, \tilde{f} \} \in T_{\max} \mid F \gamma_x(\hat{z}) + G \gamma_u(\hat{z}) = 0 \}. \quad (3.22)$$

- (ii) We have $T_{F,G} = T_{\mathcal{F},\mathcal{G}}$, where \mathcal{F}, \mathcal{G} satisfy (3.21), if and only if $\mathcal{F} = CF$ and $\mathcal{G} = CG$ for some invertible matrix $C \in \mathbb{C}^{2 \times 2}$.
- (iii) A linear relation T is a self-adjoint extension of T_{\min} if and only if there exists a unitary matrix $V \in \mathbb{C}^{2 \times 2}$ such that

$$T = T_V := \{ \{ \tilde{z}, \tilde{f} \} \in T_{\max} \mid i(V - I) \gamma_x(\hat{z}) = (V + I) \gamma_u(\hat{z}) \}. \quad (3.23)$$

- (iv) We have $T_V = T_{\mathcal{V}}$, where $\mathcal{V} \in \mathbb{C}^{2 \times 2}$ is a unitary matrix, if and only if $\mathcal{V} = V$.

Proof. (i) Let T be given by (3.22) with $F, G \in \mathbb{C}^{2 \times 2}$ satisfying (3.21). If we put $M := FP_0 + GP_{\pi/2}$ and $L := FQ_{\pi/2} + GQ_0$, where P_ω and Q_ω are the matrices corresponding to P, Q defined in (3.18) with $\omega \in \{0, \pi/2\}$. Then $M\mathcal{J}M^* - L\mathcal{J}L^* = FG^* - GF^* = 0$ and $\text{rank}(F, G) = 2$ is equivalent with $\text{rank}(M, L) = 2$. Hence M, L satisfy (3.16). Moreover, for the left-hand side of the boundary conditions in (3.22) we have $F \gamma_x(\hat{z}) + G \gamma_u(\hat{z}) = \gamma_{M,L}(\hat{z})$. Therefore $\{ \tilde{z}, \tilde{f} \} \in T_{M,L}$ if and only if $\{ \tilde{z}, \tilde{f} \} \in T_{F,G}$, i.e., $T_{F,G}$ is a self-adjoint extension of T_{\min} by Corollary 3.7. On the other hand, let T be a self-adjoint extension of T_{\min} , i.e., $T = T_{M,L}$ with $M, L \in \mathbb{C}^{2 \times 2}$ satisfying (3.16). If we put $F := MP_0 - LP_{\pi/2}$ and $G := LQ_0 - MQ_{\pi/2}$, then the conditions in (3.21) hold and $\gamma_{M,L}(\hat{z})$ can be written as in (3.22).

(ii) Sufficiency is clear. Assume that $T_{F,G} = T_{\mathcal{F},\mathcal{G}}$ for two pairs of matrices F, G and \mathcal{F}, \mathcal{G} satisfying (3.21). Then, by (3.22), we have for any $\{ \tilde{z}, \tilde{f} \} \in T_{\max}$ that $F \gamma_x(\hat{z}) + G \gamma_u(\hat{z}) = 0$ if and only if $\mathcal{F} \gamma_x(\hat{z}) + \mathcal{G} \gamma_u(\hat{z}) = 0$. It means that \hat{z}_0, \hat{z}_{N+1} solve simultaneously the both systems of algebraic equations with the coefficient matrices F, G and \mathcal{F}, \mathcal{G} . It means that these systems are equivalent, which implies an existence of an invertible matrix $C \in \mathbb{C}^{2 \times 2}$ such that $\mathcal{F} = CF$ and $\mathcal{G} = CG$.

(iii) Let T be given by (3.23) with a unitary matrix $V \in \mathbb{C}^{2 \times 2}$. If we put $F := \frac{i}{2}(I - V)$ and $G := \frac{1}{2}(I + V)$. Then $FG^* = GF^*$ and, by (2.3), $\text{rank}(F, G) = 2$, i.e., F, G satisfy (3.21). Since the boundary conditions in (3.23) are equivalent with the boundary conditions in (3.22) with F, G defined above, i.e., $\{ \tilde{z}, \tilde{f} \} \in T_{F,G}$ if and only if $\{ \tilde{z}, \tilde{f} \} \in T_V$, it follows from the previous part that the linear relation T_V is a self-adjoint extension of T_{\min} . On the other hand, let T be a self-adjoint extension of T_{\min} . Then, by the part (i), we have $T = T_{F,G}$ with $F, G \in \mathbb{C}^{2 \times 2}$ satisfying (3.21). Since by (2.3) and (3.21) we have $\text{rank}(F + iG) = 2$, the matrix $V := (F + iG)^{-1}(iG - F)$ is well-defined. One can directly verify that V is a unitary matrix and the boundary conditions $F \gamma_x(\hat{z}) + G \gamma_u(\hat{z}) = 0$ are satisfied if and only if $i(V - I) \gamma_x(\hat{z}) - (V + I) \gamma_u(\hat{z}) = 0$, i.e., $T_{F,G} = T_V$.

(iv) If $V = \mathcal{V}$, then $T_V = T_{\mathcal{V}}$. On the other hand, assume that $T_V = T_{\mathcal{V}}$ for two unitary matrices $V, \mathcal{V} \in \mathbb{C}^{2 \times 2}$. Then $T_{F,G} = T_V = T_{\mathcal{V}} = T_{\mathcal{F},\mathcal{G}}$ with F, G and \mathcal{F}, \mathcal{G} being given as in the previous part. Then $V = (F + iG)^{-1}(iG - F)$ and $\mathcal{V} = (\mathcal{F} + i\mathcal{G})^{-1}(i\mathcal{G} - \mathcal{F})$ and by the part (ii) there exists an invertible matrix $C \in \mathbb{C}^{2 \times 2}$ such that $\mathcal{F} = CF$ and $\mathcal{G} = CG$. Upon combining these facts we obtain $V = \mathcal{V}$. ■

Remark 3.12.

- (i) As a consequence of Theorem 3.9(i)-(ii) we obtain that $T_{M,L} = T_{\mathcal{M},\mathcal{L}}$ if and only if $\mathcal{M} = CM$ and $\mathcal{L} = CL$ for some invertible matrix $C \in \mathbb{C}^{2 \times 2}$.

- (ii) The statement of Theorem 3.9(iii)-(iv) shows that the map from the set of all 2×2 unitary matrices to the set of all self-adjoint extensions expressed as in (3.23) is a bijection.

4. PROOF OF MAIN RESULT

In this section, a proof is given for Theorem 3.3 which utilizes several arguments from the linear algebra and whose main idea goes back to [43]. It is based on a construction of a suitable GKN-set (see Theorem 2.11), and on a more convenient expression than that given in (3.8) for elements in $\text{dom } T_{\max}$. Similar results for system (1.4) can be found in [31, Section 4].

Lemma 4.1. *Let Hypothesis 2.4 be satisfied, $\{\tilde{z}, \tilde{f}\} \in T_{\max}$ arbitrary, and $\varphi^{[1]}, \dots, \varphi^{[q+]}$ be arranged such that (3.11) holds. Then the element \hat{z} can be uniquely expressed as*

$$\hat{z}_k = \hat{y}_k + \sum_{i=1}^{2n} \eta_i \hat{z}_k^{[i]} + \sum_{j=1}^{p-2n} \zeta_j \varphi_k^{[j]}, \quad k \in \mathcal{I}_{\mathbb{Z}}^+, \quad (4.1)$$

where $\hat{y} \in \text{dom } T_{\min}$, $\hat{z}^{[1]}, \dots, \hat{z}^{[2n]}$ are specified in Lemma 3.1, and $\eta_i, \zeta_j \in \mathbb{C}$ for all $i \in \{1, \dots, 2n\}$ and $j \in \{1, \dots, p-2n\}$. Moreover,

$$\text{rank } \Omega_{p-2n} = p - 2n, \quad (4.2)$$

where Ω was defined in (3.7).

Proof. Since (3.11) is satisfied, there exists an invertible matrix $P \in \mathbb{C}^{p \times p}$ such that

$$\Omega P = \begin{pmatrix} I_{p-2n} & 0 \\ Q & R \end{pmatrix}, \quad (4.3)$$

where I_{p-2n} is the $(p-2n) \times (p-2n)$ identity matrix and 0 stands for the $(p-2n) \times 2n$ zero matrix. If we put $\Xi = (\Xi^{[1]}, \Xi^{[2]})$, where $\Xi^{[1]} \in \mathbb{C}^{2n \times (p-2n)}$ and $\Xi^{[2]} \in \mathbb{C}^{2n \times 2n}$, and multiply (4.3) by $\bar{\Xi}$ from the left, we obtain

$$\bar{\Xi}^{[1]} = -\bar{\Xi}^{[2]} Q,$$

i.e., $\bar{\Xi} = (-\bar{\Xi}^{[2]} Q, \bar{\Xi}^{[2]})$. It implies that $\text{rank } \Xi^{[2]} = 2n$ by the second inequality in (2.2), because $\text{rank } \Xi = 2n$. By multiplying equality (3.10) by the matrix $(\Xi^{[2]})^{\top-1}$ from the right, we get

$$Z_k (\Xi^{[2]})^{\top-1} = Y_k (\Xi^{[2]})^{\top-1} + \Phi_k^{[1]} \Xi^{[1]\top} (\Xi^{[2]})^{\top-1} + \Phi_k^{[2]},$$

where $\Phi_k^{[1]} \in \mathbb{C}^{2n \times (p-2n)}$ and $\Phi_k^{[2]} \in \mathbb{C}^{2n \times 2n}$ are such that $\Phi_k = (\Phi_k^{[1]}, \Phi_k^{[2]})$. It shows that every solution $\varphi^{[2n-p+1]}, \dots, \varphi^{[p]}$ can be uniquely expressed with $\hat{y}^{[i]}, \hat{z}^{[i]}, i \in \{1, \dots, 2n\}$, and $\varphi^{[1]}, \dots, \varphi^{[p-2n]}$, i.e.,

$$\varphi_k^{[j]} = \hat{u}_k^{[j]} + \sum_{r=1}^{2n} \eta_{j,r} \hat{z}_k^{[r]} + \sum_{s=1}^{p-2n} \zeta_{j,s} \varphi_k^{[s]}, \quad k \in \mathcal{I}_{\mathbb{Z}}^+, \quad j \in \{p-2n+1, \dots, p\}, \quad (4.4)$$

for some $\hat{u}_k^{[j]} \in \text{dom } T_{\min}$ and $\eta_{j,r}, \zeta_{j,s} \in \mathbb{C}$. Therefore, the expression in (4.1) follows from (3.8). Moreover, if we multiply (4.4) by $\varphi_k^{[i]*} \mathcal{J}$ from the left, where $i \in \{1, \dots, p-2n\}$, then

$$(\varphi^{[i]}, \varphi^{[j]})_{N+1} = (\varphi^{[i]}, \hat{y}^{[j]})_{N+1} + \sum_{r=1}^{2n} \eta_{j,r} (\varphi^{[i]}, \hat{z}^{[r]})_{N+1} + \sum_{s=1}^{p-2n} \zeta_{j,s} (\varphi^{[i]}, \varphi^{[s]})_{N+1}.$$

Hence from (3.3) and the definition of $\hat{z}^{[i]}$ we have

$$\Omega_{p-2n, q-}^{[1,2]} = \Omega_{p-2n} T^{\top}, \quad (4.5)$$

where $T \in \mathbb{C}^{q_- \times (p-2n)}$ is a matrix consisting of the elements $\zeta_{j,s}$ for $j \in \{q_+ + 1, \dots, p\}$ and $s \in \{1, \dots, p - 2n\}$. Since the solutions are arranged such that $\text{rank } \Omega_{p-2n, q_-}^{[1,2]} = p - 2n$, identity (4.2) follows from (4.5) and the second inequality in (2.2). \blacksquare

Remark 4.2. If we switch the role of $v^{[1]}(\lambda_0)$ and $w^{[1]}(\bar{\lambda}_0)$ in the definition of $\varphi^{[1]}, \dots, \varphi^{[p]}$ in (3.6), i.e., we put $\varphi^{[i]} = w^{[i]}(\bar{\lambda}_0)$ for $i \in \{1, \dots, q_-\}$ and $\varphi^{[j+q_-]} = v^{[j]}(\lambda_0)$ for $j \in \{1, \dots, q_+\}$, then the solutions $\varphi^{[1]}, \dots, \varphi^{[q_-]}$ can be arranged such that (4.1) and (4.2) hold.

Now, we give the proof of Theorem 3.3.

Proof of Theorem 3.3. Assume that T is a self-adjoint extension of T_{\min} . Then, by Theorem 2.11 there exists a GKN-set $\{\beta_j\}_{j=1}^q$ for (T_{\min}, T_{\max}) such that (2.38) holds. Since $\beta_j \in T_{\max}$, they may be identified as $\beta_j = \{\tilde{w}^{[j]}, \tilde{h}^{[j]}\} \in T_{\max}$. By Lemma 4.1, the elements $\hat{w}^{[j]}$ can be uniquely expressed as

$$\hat{w}_k^{[j]} = \hat{y}_k^{[j]} + \sum_{i=1}^{2n} \eta_{j,i} \hat{z}_k^{[i]} + \sum_{l=1}^{2q-2n} \zeta_{j,l} \varphi_k^{[l]}, \quad k \in \mathcal{I}_{\mathbb{Z}}^+, \quad (4.6)$$

where $\hat{y}^{[j]} \in \text{dom } T_{\min}$ and $\eta_{j,i}, \zeta_{j,l} \in \mathbb{C}$. We next show that the matrices

$$M := (\hat{w}_0^{[1]}, \dots, \hat{w}_0^{[q]})^* \mathcal{J} \in \mathbb{C}^{q \times 2n}, \quad L := \begin{pmatrix} \overline{\zeta_{1,1}} & \cdots & \overline{\zeta_{1,2q-2n}} \\ \vdots & \ddots & \vdots \\ \overline{\zeta_{q,1}} & \cdots & \overline{\zeta_{q,2q-2n}} \end{pmatrix} \in \mathbb{C}^{q \times (2q-2n)}$$

satisfy (3.12).

Since $\text{rank}(M, L) \leq q$, assume that $\text{rank}(M, L) < q$. Then, there exists $C = (c_1, \dots, c_q)^\top \in \mathbb{C}^q \setminus \{0\}$ such that $C^*(M, L) = 0$, i.e., $C^*M = 0 = C^*L$. If $\hat{w}_k := \sum_{j=1}^q c_j \hat{w}_k^{[j]}$ for $k \in \mathcal{I}_{\mathbb{Z}}^+$, then $\hat{w}_0 = \mathcal{J}M^*C = 0$ and also $(\hat{w}, \varphi^{[i]})_{N+1} = \sum_{j=1}^q \overline{c_j} (\hat{w}^{[j]}, \varphi^{[i]})_{N+1}$ for all $i \in \{1, \dots, 2q - 2n\}$. Hence by (4.6) and (3.3) we have

$$((\hat{w}, \varphi^{[1]})_{N+1}, \dots, (\hat{w}, \varphi^{[2q-2n]})_{N+1}) = C^*L \Omega_{2q-2n} = 0.$$

But then $(\hat{w}, \hat{y})_{N+1} = 0$ for any $\hat{y} \in \text{dom } T_{\max}$, because it can be written as in (4.1). It means that $\hat{w} \in \text{dom } T_{\min}$ by (3.3) and hence β_1, \dots, β_q are linearly dependent in T_{\max} modulo T_{\min} , which contradicts the assumption that $\{\beta_j\}_{j=1}^q$ is a GKN-set. Therefore, the first condition in (3.12) is satisfied.

Next, we see that

$$\begin{pmatrix} (\hat{w}^{[1]}, \hat{w}^{[1]})_0 & \cdots & (\hat{w}^{[1]}, \hat{w}^{[q]})_0 \\ \vdots & \ddots & \vdots \\ (\hat{w}^{[q]}, \hat{w}^{[1]})_0 & \cdots & (\hat{w}^{[q]}, \hat{w}^{[q]})_0 \end{pmatrix} = M \mathcal{J} M^* \quad (4.7)$$

and by using (4.6), (3.3), and the definition of $\hat{z}^{[i]}$, also see that

$$\begin{pmatrix} (\hat{w}^{[1]}, \hat{w}^{[1]})_{N+1} & \cdots & (\hat{w}^{[1]}, \hat{w}^{[q]})_{N+1} \\ \vdots & \ddots & \vdots \\ (\hat{w}^{[q]}, \hat{w}^{[1]})_{N+1} & \cdots & (\hat{w}^{[q]}, \hat{w}^{[q]})_{N+1} \end{pmatrix} = L \Omega_{2q-2n} L^*. \quad (4.8)$$

Since $\{\beta_j\}_{j=1}^q$ is a GKN-set, we obtain from (3.1) that

$$0 = [\beta_i : \beta_j] = (\hat{w}^{[i]}, \hat{w}^{[j]})_k \Big|_0^{N+1}$$

for all $i, j \in \{1, \dots, q\}$. By (4.7) and (4.8), this implies that $M\mathcal{J}M^* - L\Omega_{2q-2n}L^* = 0$, and that the second condition in (3.12) is also satisfied.

For any $\hat{z} \in \text{dom } T_{\max}$, we can write

$$\begin{pmatrix} (\hat{w}^{[1]}, \hat{z})_0 \\ \vdots \\ (\hat{w}^{[q]}, \hat{z})_0 \end{pmatrix} = M\hat{z}_0, \quad \begin{pmatrix} (\hat{w}^{[1]}, \hat{z})_{N+1} \\ \vdots \\ (\hat{w}^{[q]}, \hat{z})_{N+1} \end{pmatrix} = L \begin{pmatrix} (\varphi^{[1]}, \hat{z})_{N+1} \\ \vdots \\ (\varphi^{[2q-2n]}, \hat{z})_{N+1} \end{pmatrix}, \quad (4.9)$$

where the second equality follows from (4.6), (3.3), and the definition of $\hat{z}^{[i]}$. Upon combining (2.38), (3.1), (4.9), we obtain that T can be expressed as

$$\begin{aligned} T &= \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid (\hat{z}, \hat{w}^{[j]})_k \Big|_0^{N+1} = 0 \text{ for all } j = 1, \dots, q \right\} \\ &= \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid \hat{w}_k^{[j]*} \mathcal{J} \hat{z}_k \Big|_0^{N+1} = 0 \text{ for all } j = 1, \dots, q \right\} \\ &= \left\{ \{\tilde{z}, \tilde{f}\} \in T_{\max} \mid M\hat{z}_0 - L \begin{pmatrix} (\varphi^{[1]}, \hat{z})_{N+1} \\ \vdots \\ (\varphi^{[2q-2n]}, \hat{z})_{N+1} \end{pmatrix} = 0 \right\}, \end{aligned}$$

i.e., as written in (3.13).

On the other hand, let $M \in \mathbb{C}^{q \times 2n}$ and $L \in \mathbb{C}^{q \times (2q-2n)}$ satisfy (3.12) and T be given by (3.13). We then must show that there exists a GKN-set $\{\beta_j\}_{j=1}^q$ for (T_{\min}, T_{\max}) such that T can be expressed as in (2.38). Denote the columns of $\mathcal{J}M^* \in \mathbb{C}^{2n \times q}$ as ρ_1, \dots, ρ_q and the columns of the matrix $(\varphi_k^{[1]}, \dots, \varphi_k^{[2q-2n]}) L^* \in \mathbb{C}^{2n \times q}$ as $w_k^{[1]}, \dots, w_k^{[q]}$, i.e.,

$$\rho_i := \mathcal{J}M^* e_i, \quad w_k^{[i]} := \sum_{l=1}^{2q-2n} \overline{\eta_{i,l}} \varphi_k^{[l]}, \quad i \in \{1, \dots, q\}, \quad (4.10)$$

where e_i is the i -th canonical unit vector in \mathbb{C}^q and $\eta_{i,j}$ are the elements of L for $i \in \{1, \dots, q\}$ and $j \in \{1, \dots, 2q-2n\}$. Then, $w_k^{[i]} \in T_{\max}$ for all $i \in \{1, \dots, q\}$ and, by Lemma 3.1, there exist $\beta_i := \{\tilde{y}^{[i]}, \tilde{h}^{[i]}\} \in T_{\max}$ such that

$$\hat{y}_0^{[i]} = \rho_i, \quad \hat{y}_k^{[i]} = w_k^{[i]}, \quad k \in [b+1, \infty)_{\mathbb{Z}} \cap \mathcal{I}_{\mathbb{Z}}^+$$

for all $i \in \{1, \dots, q\}$, where the number b is determined in Hypothesis 2.4. We next show that $\{\beta_i\}_{i=1}^q$ form a GKN-set for (T_{\min}, T_{\max}) .

Since the linear independence of β_1, \dots, β_q in T_{\max} modulo T_{\min} is equivalent to the linear independence of $\hat{y}^{[1]}, \dots, \hat{y}^{[q]}$ in $\text{dom } T_{\max}$ modulo T_{\min} , we assume that there exists $C = (c_1, \dots, c_q)^{\top} \in \mathbb{C}^q \setminus \{0\}$ such that

$$\hat{y} := \sum_{j=1}^q c_j \hat{y}^{[j]} \in \text{dom } T_{\min}.$$

Then, from (3.3) and (4.10), we have for all $\varphi^{[1]}, \dots, \varphi^{[2q-2n]} \in T_{\max}$ that

$$0 = ((\hat{y}, \varphi^{[1]})_{N+1}, \dots, (\hat{y}, \varphi^{[2q-2n]})_{N+1}) = C^* L \Omega_{2q-2n}.$$

This implies $C^* L = 0$, because Ω_{2q-2n} is assumed to be invertible. Simultaneously we have $\hat{y}_0 = 0$, which yields

$$0 = \hat{y}_0 = \sum_{j=1}^q c_j \hat{y}_0^{[j]} = \mathcal{J}M^* C,$$

i.e., $C^*M = 0$, because the matrix \mathcal{J} is invertible. But this means $C^*(M, L) = 0$, which contradicts the first assumption in (3.12).

Next, let

$$Y_k := \begin{pmatrix} (\hat{y}^{[1]}, \hat{y}^{[1]})_k & \cdots & (\hat{y}^{[1]}, \hat{y}^{[q]})_k \\ \vdots & \ddots & \vdots \\ (\hat{y}^{[q]}, \hat{y}^{[1]})_k & \cdots & (\hat{y}^{[q]}, \hat{y}^{[q]})_k \end{pmatrix}.$$

Since it can be directly calculated that $Y_0 = M\mathcal{J}M^*$ and $Y_{N+1} = L\Omega_{2q-2n}L^*$, the second equality in (3.12) implies $Y_0 - Y_{N+1} = 0$. Therefore, by using (3.1), we get

$$[\beta_i : \beta_j] = (\hat{y}^{[i]}, \hat{y}^{[j]})_k \Big|_0^{N+1} = 0,$$

which shows that $\{\beta_i\}_{i=1}^q$ is a GKN-set for (T_{\min}, T_{\max}) as defined in Subsection 2.2.

Finally, let $\{\tilde{w}, \tilde{g}\} \in T_{\max}$ be arbitrary, then

$$M\hat{w}_0 = \begin{pmatrix} (\hat{y}^{[1]}, \hat{w})_0 \\ \vdots \\ (\hat{y}^{[q]}, \hat{w})_0 \end{pmatrix}, \quad L \begin{pmatrix} (\varphi^{[1]}, \hat{w})_{N+1} \\ \vdots \\ (\varphi^{[2q-2n]}, \hat{w})_{N+1} \end{pmatrix} = \begin{pmatrix} (\hat{y}^{[1]}, \hat{w})_{N+1} \\ \vdots \\ (\hat{y}^{[q]}, \hat{w})_{N+1} \end{pmatrix}. \quad (4.11)$$

By (3.1) the condition $[\{\tilde{w}, \tilde{g}\} : \beta_i] = 0$ is equivalent to

$$(\hat{w}, \hat{y}^{[i]})_k \Big|_0^{N+1} = 0 = -(\hat{y}^{[i]}, \hat{w})_k \Big|_0^{N+1} \quad (4.12)$$

for all $i \in \{1, \dots, q\}$. Hence, by (4.11), we see that (4.12) can be written as

$$M\hat{w}_0 - L \begin{pmatrix} (\varphi^{[1]}, \hat{w})_{N+1} \\ \vdots \\ (\varphi^{[2q-2n]}, \hat{w})_{N+1} \end{pmatrix} = 0.$$

Therefore, the linear relation T in (3.13) can be equivalently expressed as in (2.38), which means that T is a self-adjoint extension of T_{\min} . \blacksquare

The simplification of Theorem 3.3 in the limit circle case is based on the following lemma.

Lemma 4.3. *Let Hypothesis 2.4 be satisfied and $\varphi^{[1]}, \dots, \varphi^{[q+]}$ be arranged as in Lemma 4.1. Assume that there exists $\nu \in \mathbb{R}$ such that system (S_ν) has $r := \max\{q_+, q_-\}$ linearly independent square summable solutions (suppressing the argument ν) given by $\Theta^{[1]}, \dots, \Theta^{[r]}$. Then these solutions can be arranged such that $\text{rank } \Upsilon_{p-2n} = p - 2n$, where*

$$\Upsilon := \begin{pmatrix} (\Theta^{[1]}, \Theta^{[1]})_{N+1} & \cdots & (\Theta^{[1]}, \Theta^{[r]})_{N+1} \\ \vdots & \ddots & \vdots \\ (\Theta^{[r]}, \Theta^{[1]})_{N+1} & \cdots & (\Theta^{[r]}, \Theta^{[r]})_{N+1} \end{pmatrix} \in \mathbb{C}^{r \times r}.$$

Moreover, for any $\{\tilde{z}, \tilde{f}\} \in T_{\max}$ the element \hat{z} can be uniquely expressed as

$$\hat{z}_k = \hat{y}_k + \sum_{i=1}^{2n} \alpha_i \hat{z}_k^{[i]} + \sum_{j=1}^{p-2n} \beta_j \Theta_k^{[j]}, \quad k \in \mathbb{I}_{\mathbb{Z}}^+,$$

where $\hat{y} \in \text{dom } T_{\min}$, $\hat{z}^{[1]}, \dots, \hat{z}^{[2n]}$ are given in Lemma 3.1, and $\alpha_i, \beta_j \in \mathbb{C}$ for all $i \in \{1, \dots, 2n\}$ and $j \in \{1, \dots, p - 2n\}$.

Proof. Since $\Theta_k^{[1]}, \dots, \Theta_k^{[r]} \in \text{dom } T_{\max}$, by Lemma 4.1 there exist unique $\alpha_{i,j}, \beta_{i,l} \in \mathbb{C}$ such that

$$\Theta_k^{[i]} = \hat{y}_k^{[i]} + \sum_{j=1}^{2n} \alpha_{i,j} \hat{z}_k^{[j]} + \sum_{l=1}^{p-2n} \beta_{i,l} \varphi_k^{[l]}, \quad k \in \mathcal{I}_{\mathbb{Z}}^+, \quad (4.13)$$

where $i \in \{1, \dots, r\}$. Then, the definition of $\hat{z}_k^{[i]}$ and identity (3.3) yield

$$\Upsilon = B \Omega_{p-2n} B^*, \quad (4.14)$$

where the matrix $B = [\overline{\beta_{i,j}}] \in \mathbb{C}^{r \times (p-2n)}$. Hence, $\text{rank } \Upsilon \leq p - 2n$ by the first inequality in (2.2). On the other hand, by the Wronskian-type identity in (2.7) we have $\Upsilon = \Theta_0^* \mathcal{J} \Theta_0$, where $\Theta_k := (\Theta_k^{[1]}, \dots, \Theta_k^{[r]})$. Since the solutions $\Theta_k^{[1]}, \dots, \Theta_k^{[r]}$ are linearly independent, we have $\text{rank } \Theta_k = r$ for all $k \in \mathcal{I}_{\mathbb{Z}}^+$, and hence $\text{rank } \Upsilon \geq p - 2n$ by the second inequality in (2.2). Therefore $\text{rank } \Upsilon = p - 2n$, which implies that the solutions $\Theta_k := (\Theta_k^{[1]}, \dots, \Theta_k^{[r]})$ can be arranged such that $\text{rank } \Upsilon_{p-2n} = p - 2n$. In this case, the invertibility of B_{p-2n} follows from the equality $\Upsilon_{p-2n} = B_{p-2n} \Omega_{p-2n} B_{p-2n}^*$, which is obtained analogously to (4.14). Since from (4.13) we have

$$(\Theta_k^{[1]}, \dots, \Theta_k^{[p-2n]}) = (\hat{y}_k^{[1]}, \dots, \hat{y}_k^{[p-2n]}) + (\hat{z}_k^{[1]}, \dots, \hat{z}_k^{[2n]}) A_{2n,p-2n}^* + (\varphi_k^{[1]}, \dots, \varphi_k^{[p-2n]}) B_{q-2n}^*,$$

where $A = [\overline{\alpha_{i,j}}] \in \mathbb{C}^{r \times 2n}$, the invertibility of B_{p-2n} means that $\varphi_k^{[1]}, \dots, \varphi_k^{[p-2n]}$ can be uniquely expressed by using $\Theta_k^{[1]}, \dots, \Theta_k^{[p-2n]}, \hat{y}_k^{[1]}, \dots, \hat{y}_k^{[p-2n]}$, and $\hat{z}_k^{[1]}, \dots, \hat{z}_k^{[2n]}$. Upon combining these expressions with (4.1), we obtain the second part of the statement. ■

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